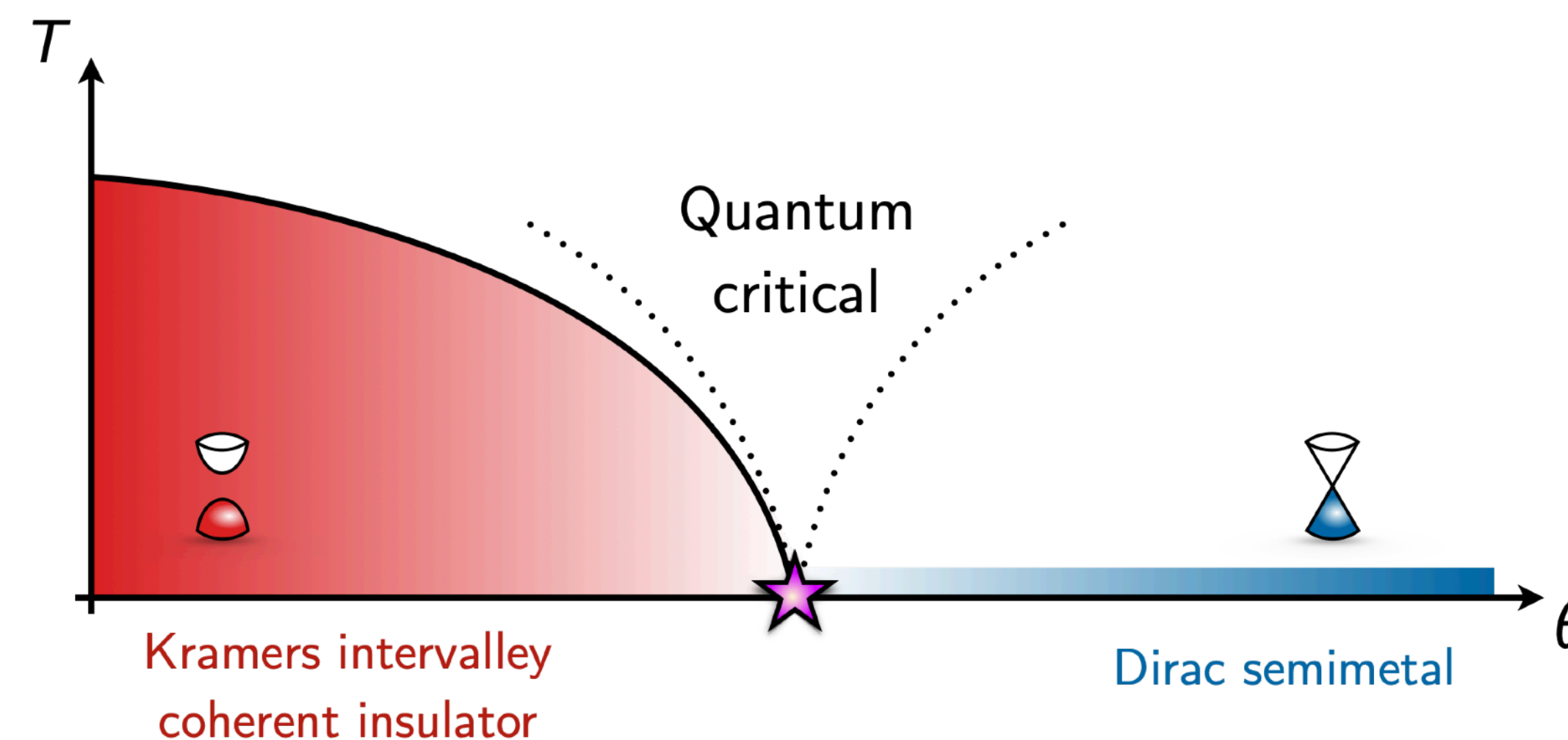


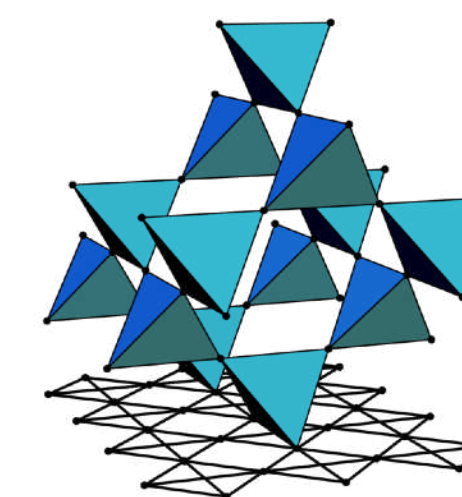
Twist-tuned quantum criticality in bilayer graphene

Jan Biedermann & Lukas Janssen



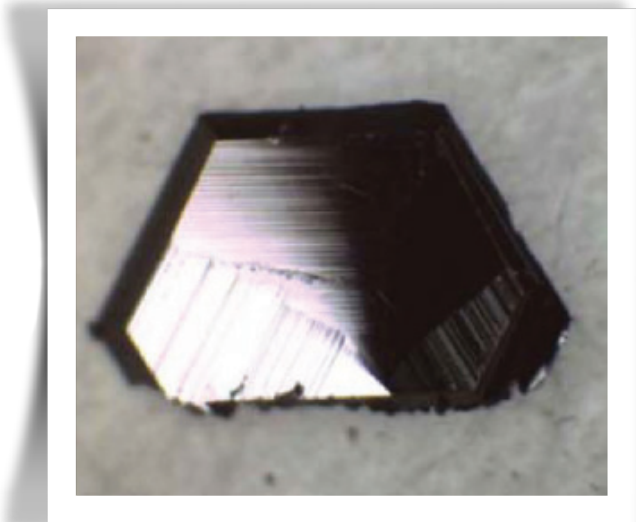
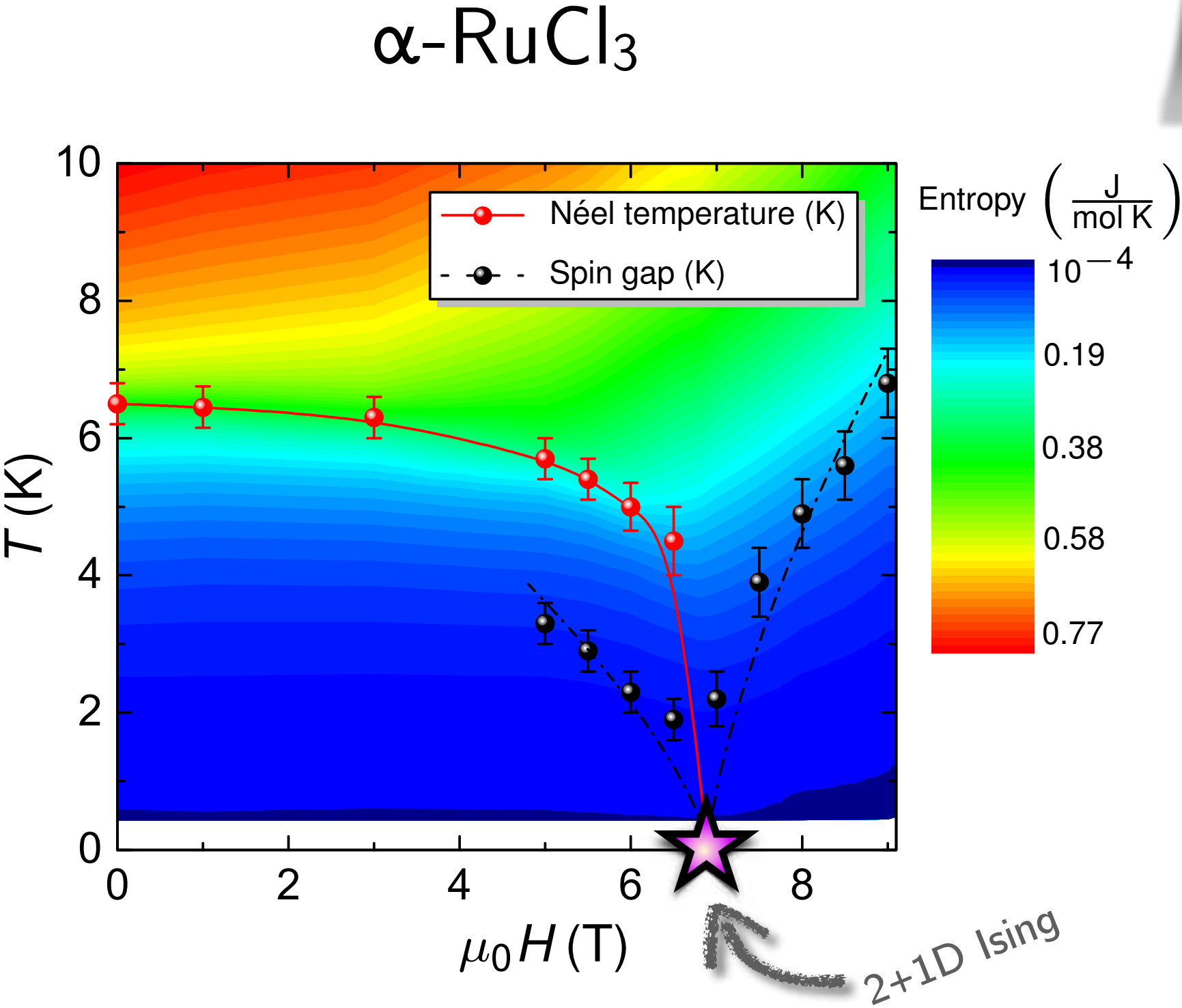
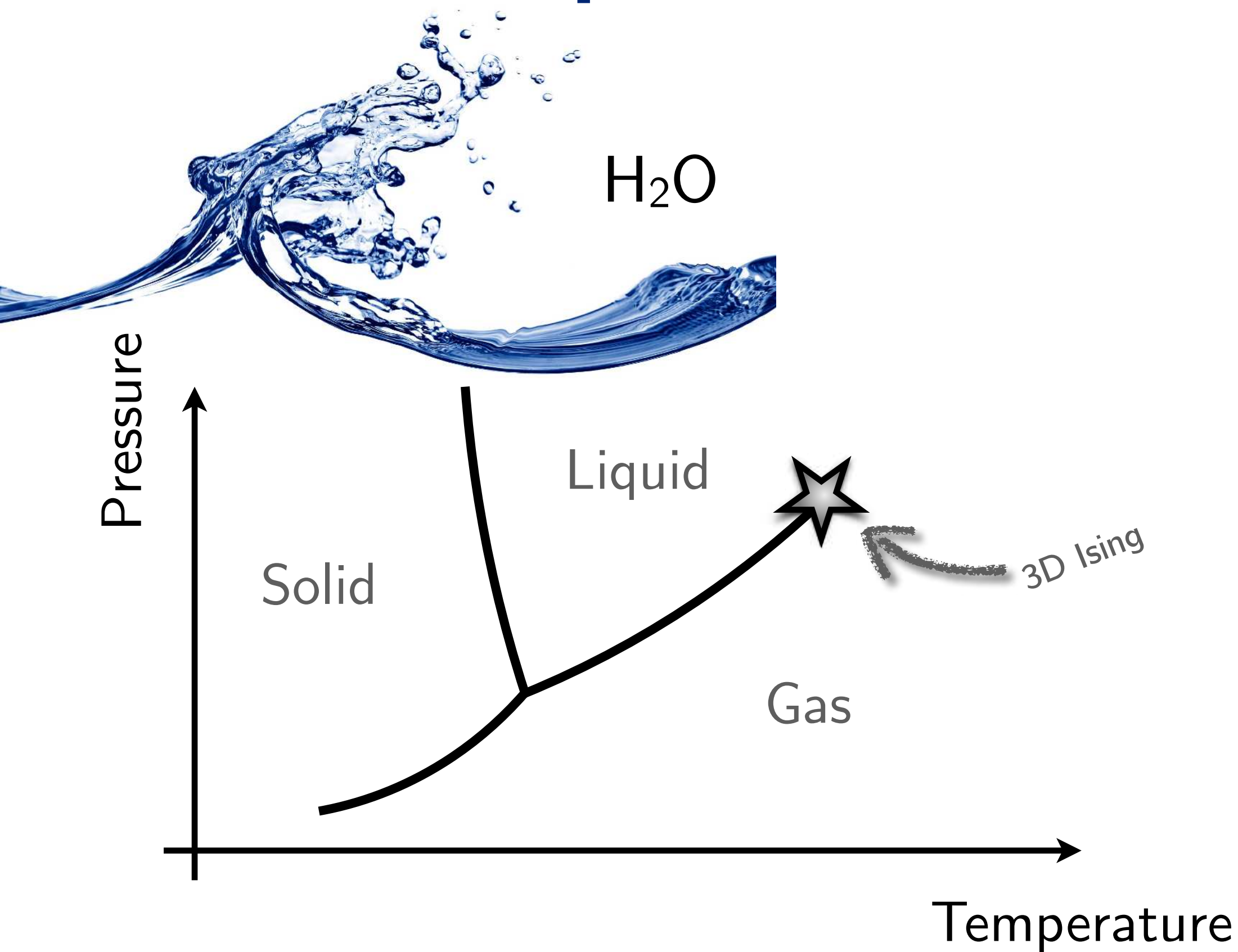
ct.qmat
Complexity and Topology
in Quantum Matter

Würzburg-Dresden Cluster of Excellence



SFB 1143

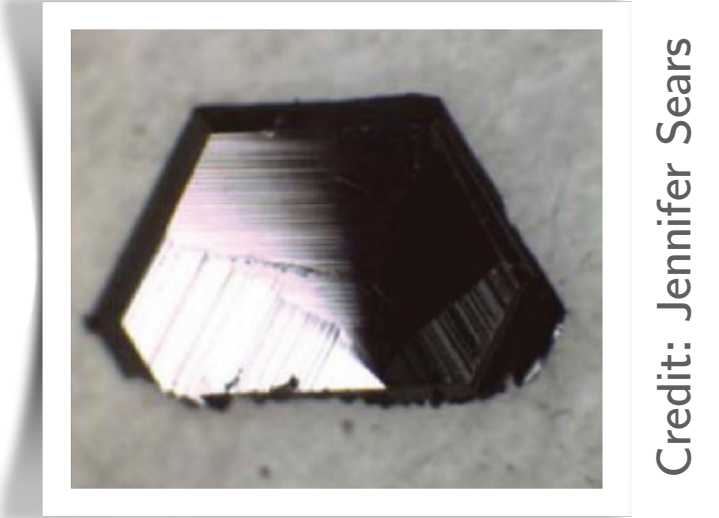
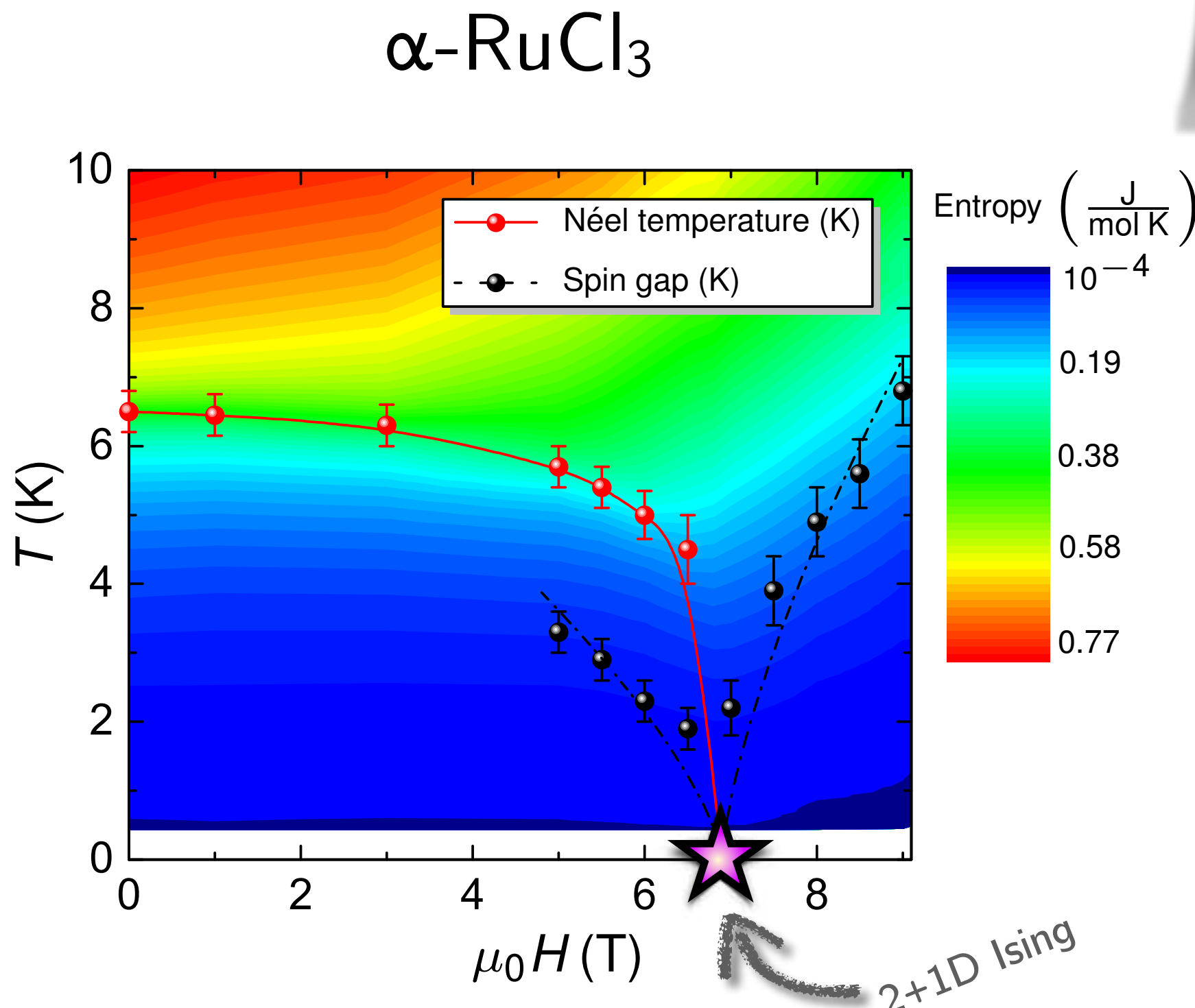
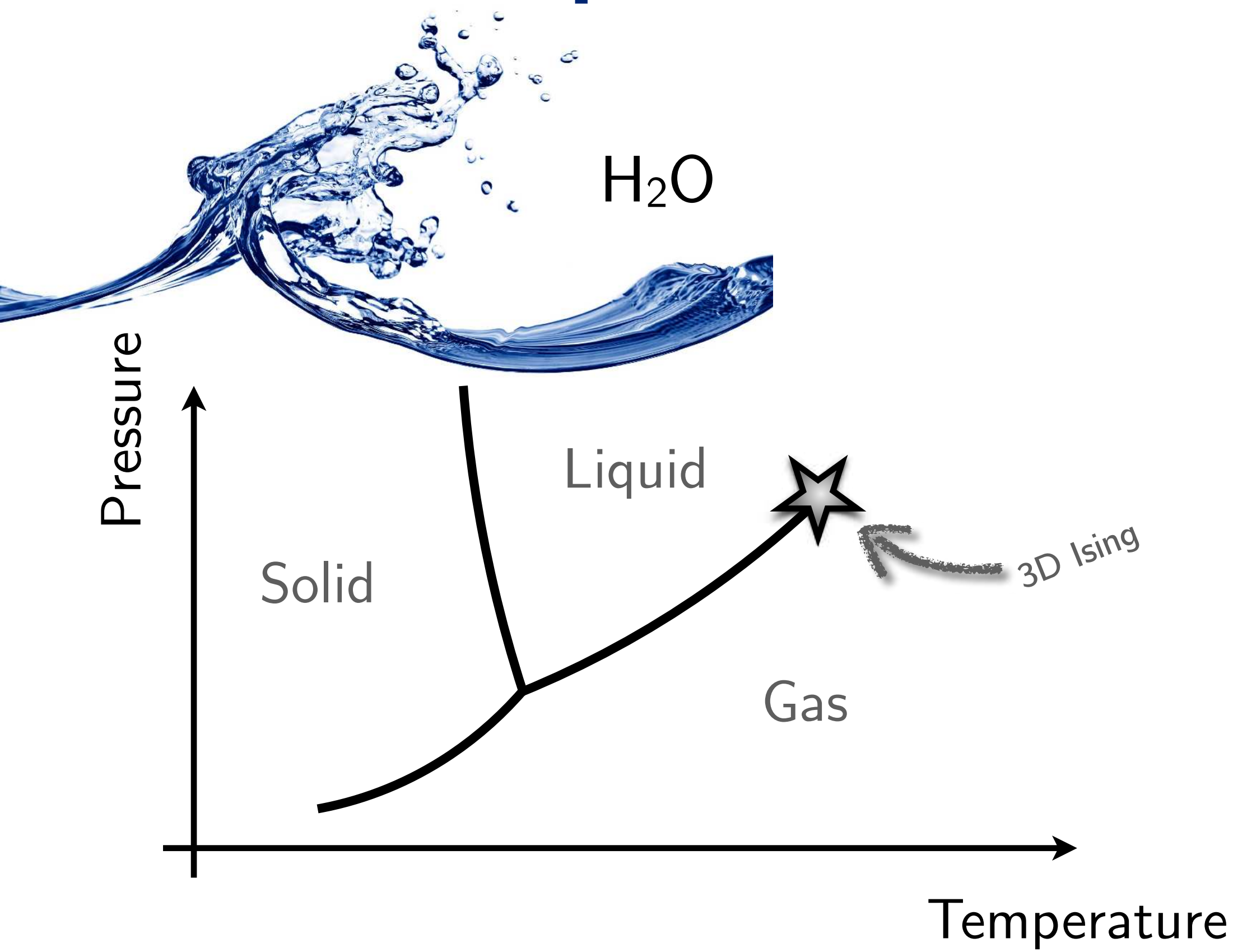
Classical vs quantum criticality



Credit: Jennifer Sears

[Wolter, Corredor, LJ, et al., PRB '17]

Classical vs quantum criticality



Credit: Jennifer Sears

[Wolter, Corredor, LJ, et al., PRB '17]

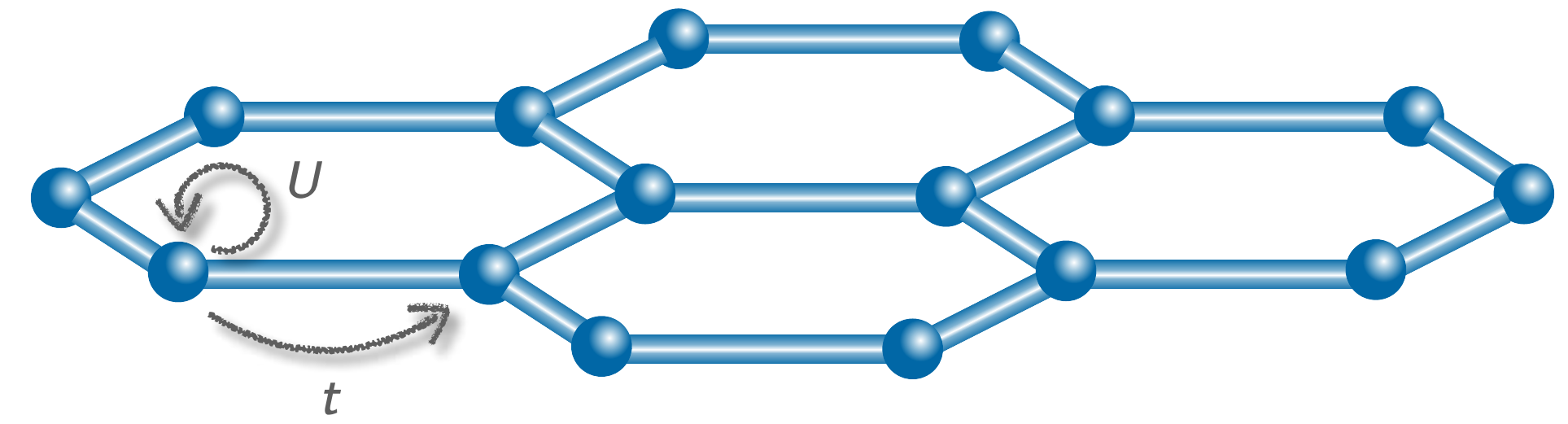
Universal field theory:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)^2 + \frac{r}{2}\phi^2 + \lambda\phi^4$$

Fermionic quantum criticality

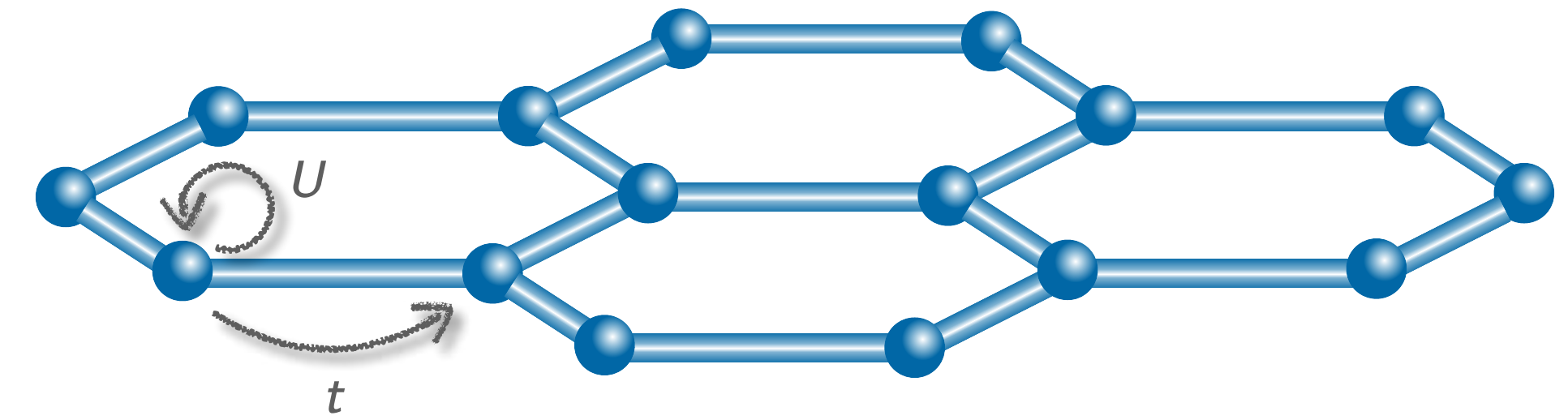
Honeycomb-lattice Hubbard model:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



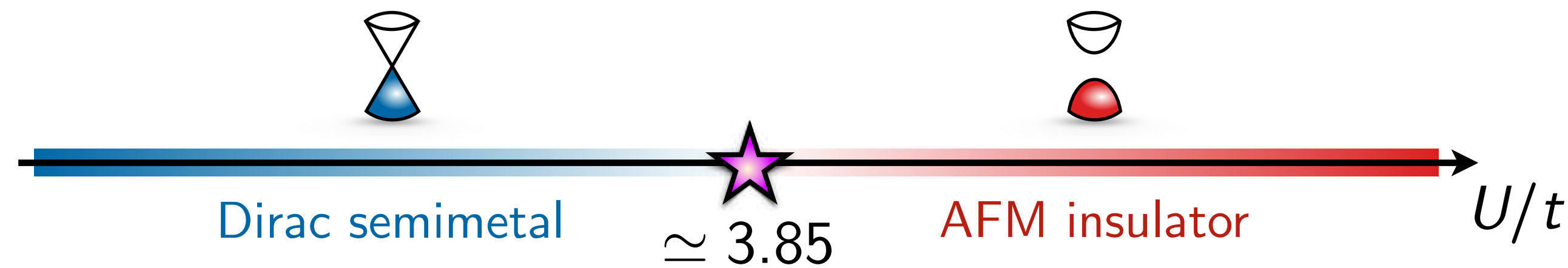
Fermionic quantum criticality

Honeycomb-lattice Hubbard model:



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Quantum phase diagram:



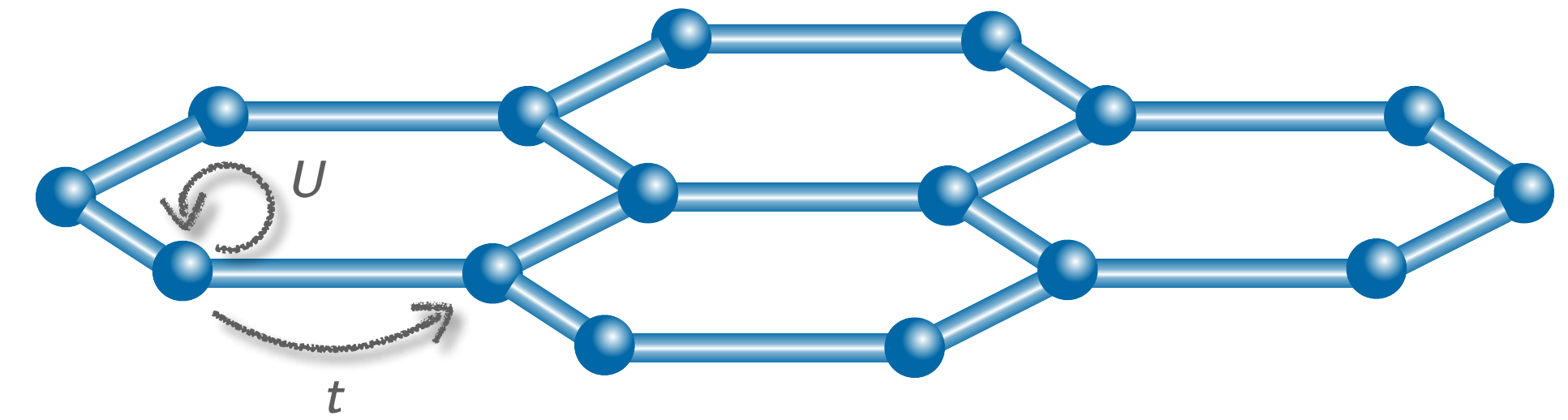
[Assaad & Herbut, PRX '13]
[Otsuka, Yunoki, Sorella, PRX '16]

→ Talk by I. Herbut

→ Talk by K. Le Hur

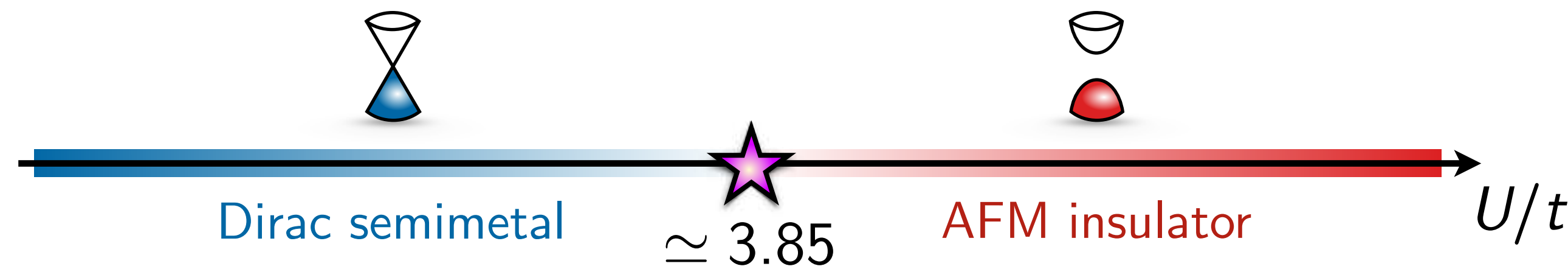
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Quantum phase diagram:



[Assaad & Herbut, PRX '13]
[Otsuka, Yunoki, Sorella, PRX '16]

→ Talk by I. Herbut

→ Talk by K. Le Hur

Gross-Neveu-Heisenberg field theory:

$$\mathcal{L} = \bar{\psi} \gamma^\mu \partial_\mu \psi + g(\bar{\psi} \vec{\sigma} \psi)^2$$

[Herbut, Juričić, Vafek, PRB '09]
[LJ, Herbut, PRB '14]
[Zerf *et al.*, PRD '17]

Experimental realization?

026802 (2009)

PHYSICAL REVIEW LETTERS

week ending
16 JANUARY 2009

Is Graphene in Vacuum an Insulator?

Joaquín E. Drut¹ and Timo A. Lähde²

¹Department of Physics, The Ohio State University, Columbus, Ohio 43210-1117, USA
²Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA

(Received 11 July 2008; published 13 January 2009)

We present evidence, from lattice Monte Carlo simulations of the phase diagram of graphene as a function of the Coulomb coupling between quasiparticles, that graphene in vacuum is likely to be an insulator. We find a semimetal-insulator transition at $\alpha_g^{\text{crit}} = 1.11 \pm 0.06$, where $\alpha_g \simeq 2.16$ in vacuum, and $\alpha_g \simeq 0.79$ on a SiO₂ substrate. Our analysis uses the logarithmic derivative of the order parameter, supplemented by an equation of state. The insulating phase disappears above a critical number of four-component fermion flavors $4 < N_f^{\text{crit}} < 6$. Our data are consistent with a second-order transition.

PACS numbers: 73.63.Bd, 05.10.Ln, 71.30.+h

DOI: [10.1103/PhysRevLett.102.026802](https://doi.org/10.1103/PhysRevLett.102.026802)

Graphene, a carbon allotrope with a two-dimensional honeycomb structure, has become an important player at the forefront of condensed matter physics, drawing the attention of theorists and experimentalists alike due to its challenging nature as a many-body problem, its unusual electronic properties, and possible technological applications (see Refs. [1,2] and references therein). Graphene also belongs to a large class of planar condensed matter systems, which includes other graphite-related materials as well as high- T_c superconductors.

A distinctive feature of graphene is that its band structure generate “Dirac points,” in the vicinity of which the quasiparticles behave as relativistic Dirac fermions. These properties resemble QED in a very strongly coupled regime. This provides an exciting opportunity for the study of strongly coupled theories, within a condensed matter analogue that can be experimentally realized with modest equipment.

Notably, Eq. (1) satisfies a chiral $U(2N_f)$ symmetry which can break spontaneously at large enough Coulomb coupling, generating a gap in the quasiparticle spectrum. Whether such an effect occurs in real graphene is an open issue from the experimental point of view (see, however, Ref. [4], where a substrate-induced gap is reported). On the theoretical side, dynamical gap generation is described by a quantum phase transition due to the formation of particle-hole bound states. However, in such a strongly coupled system, even a qualitative analysis should be nonperturbative. The situation for graphene in vacuum, where the Coulomb interaction is partially screened

Experimental realization?

1026802 (2009)

PHYSICAL REVIEW LETTERS

Is Graphene in Vacuum an Insulator?

Joaquín E. Drut¹ and Timo A. Lähde²

¹Department of Physics, The Ohio State University, Columbus, Ohio 43210
²Department of Physics, University of Washington, Seattle, Washington 98195

(Received 11 July 2008; published 13 January 2009)

We present evidence, from lattice Monte Carlo simulations, that the Coulomb coupling between Dirac fermions in vacuum is strong enough to drive a transition from a semimetal to an insulator. We find a semimetal-insulator transition at $\alpha_g \approx 0.79$ on a SiO_2 substrate. Our results are supplemented by an equation of state for the component fermion flavors $4 < N_f < 6$.

DOI: [10.1103/PhysRevLett.102.026802](https://doi.org/10.1103/PhysRevLett.102.026802)

Graphene, a carbon allotrope with a two-dimensional honeycomb structure, has become an important area of research in condensed matter physics. The attention of theorists and experimentalists has been drawn to its unique electronic properties, and possible technological applications (see Refs. [1,2] and references therein). It also belongs to a large class of planar systems, which includes other graphite-based systems, as well as high- T_c superconductors. A distinctive feature of graphene is the presence of Dirac fermions, which are massless and move at the speed of light. This property is responsible for many of its unique electronic and optical properties. In this paper, we present evidence from lattice Monte Carlo simulations that the Coulomb coupling between Dirac fermions in vacuum is strong enough to drive a transition from a semimetal to an insulator. We find a semimetal-insulator transition at $\alpha_g \approx 0.79$ on a SiO_2 substrate. Our results are supplemented by an equation of state for the component fermion flavors $4 < N_f < 6$.

PRL 115, 186602 (2015)

PHYSICAL REVIEW LETTERS

Interaction-Driven Metal-Insulator Transition in Strained Graphene

Ho-Kin Tang,^{1,2} E. Laksono,^{1,2} J. N. B. Rodrigues,^{1,2} P. Sengupta,^{1,3} F. F. Assaad,⁴ and S. Adam^{1,2,5}

¹Centre for Advanced 2D Materials, National University of Singapore, 6 Science Drive 2, Singapore 117546, Singapore
²Department of Physics, Faculty of Science, National University of Singapore, 2 Science Drive 3, Singapore 117542, Singapore
³School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371, Singapore
⁴Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany
⁵Yale-NUS College, 16 College Avenue West, Singapore 138527

(Received 28 May 2015; published 11 November 2015)

RESEARCH

RESEARCH ARTICLE

2D MATERIALS

The role of electron-electron interactions in two-dimensional Dirac fermions

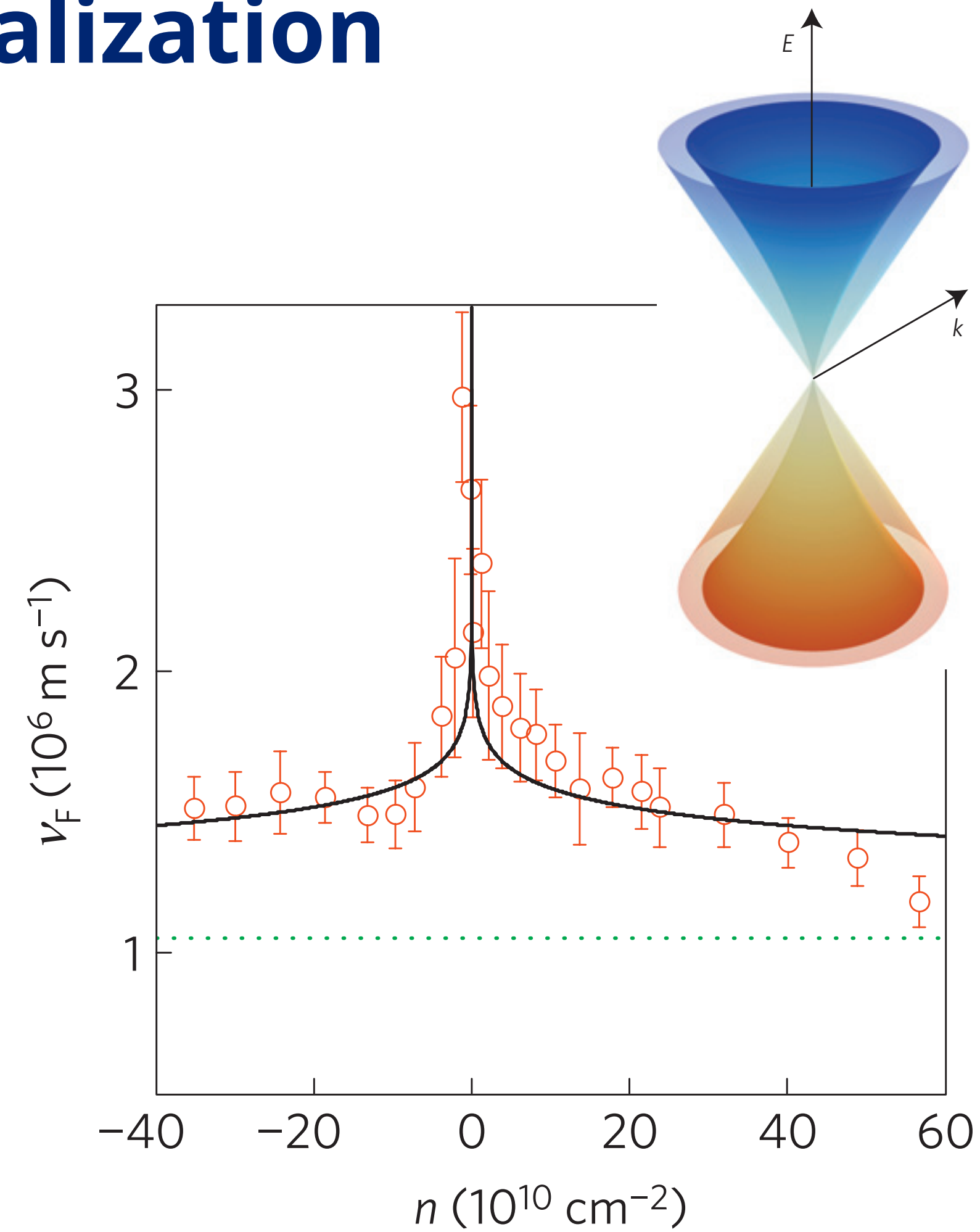
Ho-Kin Tang^{1,2}, J. N. Leaw^{1,2}, J. N. B. Rodrigues^{1,2}, I. F. Herbut³, P. Sengupta^{1,4}, F. F. Assaad⁵, S. Adam^{1,2,6*}

The role of electron-electron interactions in two-dimensional Dirac fermion systems remains enigmatic. Using a combination of nonperturbative numerical and analytical techniques that incorporate both the contact and long-range parts of the Coulomb interaction, we identify the two previously discussed regimes: a Gross-Neveu transition to a strongly correlated Mott insulator and a semimetallic state with a diverging Fermi velocity accurately predicted by the Dirac equation.

(6, 12) that this pure on-site Hubbard model has limited applicability to experiments done in real materials.

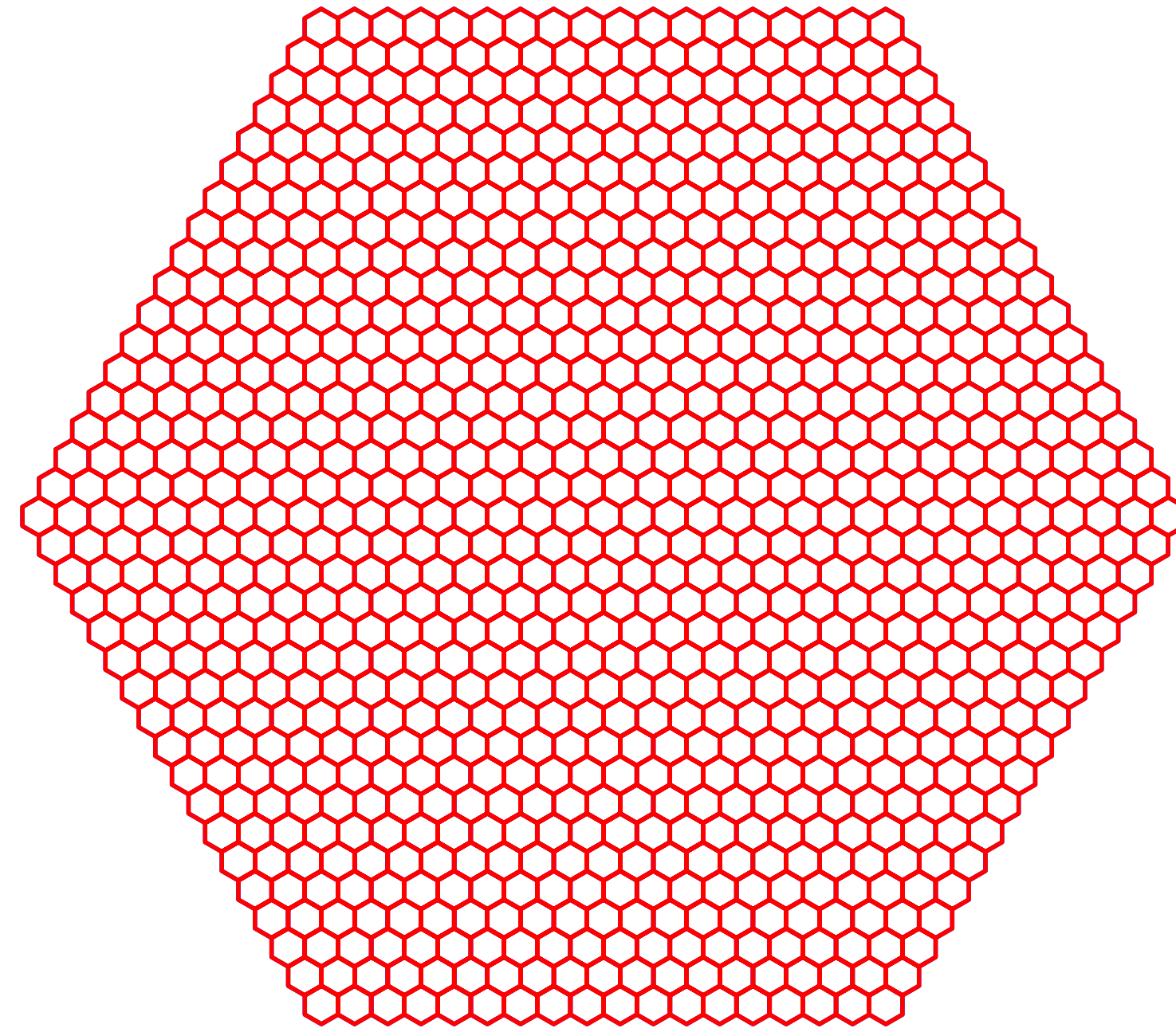
Experimentally, 2D Dirac fermions can be realized in a variety of condensed matter systems, including on the surfaces of 3D topological insulators (13, 14) and in artificial graphene made from quantum corrals of carbon monoxide arranged in a honeycomb lattice on a copper substrate (15), as well as in other systems (16). For concreteness, we focus our attention on graphene, the most studied and versatile realization of 2D Dirac fermions. Experiments have been unable to realize the precise configuration necessary to probe this strange interacting metallic state that features electron quasiparticles moving at the speed of light, despite their quasiparticle character smearing away; however, several probes of ultraclean graphene—including magnetotransport (17), infrared spectroscopy (18), and scanning tunneling spectroscopy (19)—have shown that the Dirac fermions are indeed present and short-range interactions play a crucial role in the ground state. The theoretical prediction of a semimetal-insulator transition in graphene is a long-standing open question. In this paper, we present evidence from lattice Monte Carlo simulations that the Coulomb coupling between Dirac fermions in vacuum is strong enough to drive a transition from a semimetal to an insulator. We find a semimetal-insulator transition at $\alpha_g \approx 0.79$ on a SiO_2 substrate. Our results are supplemented by an equation of state for the component fermion flavors $4 < N_f < 6$.

Fermi velocity renormalization

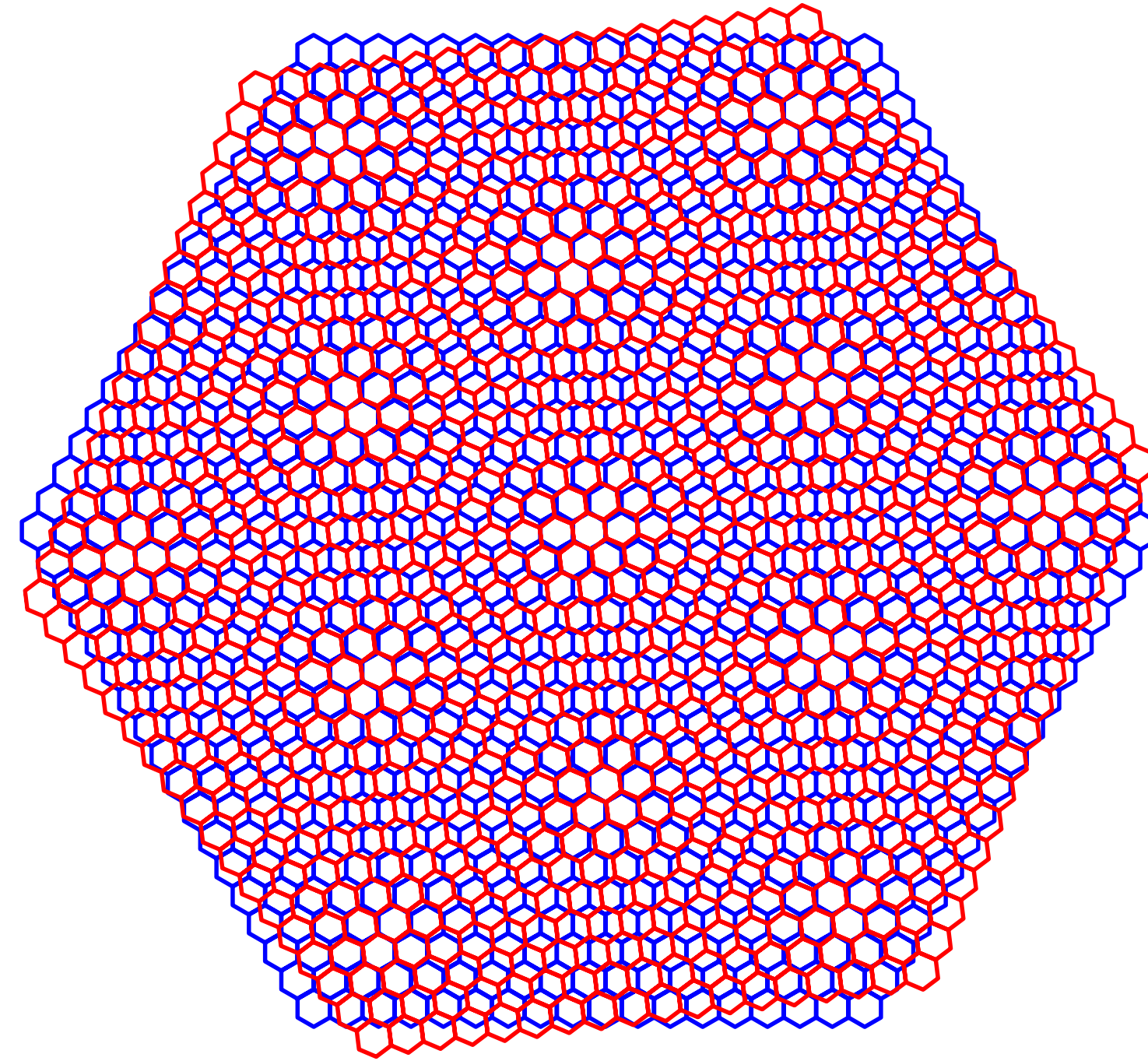


Free-standing graphene remains a Dirac semimetal

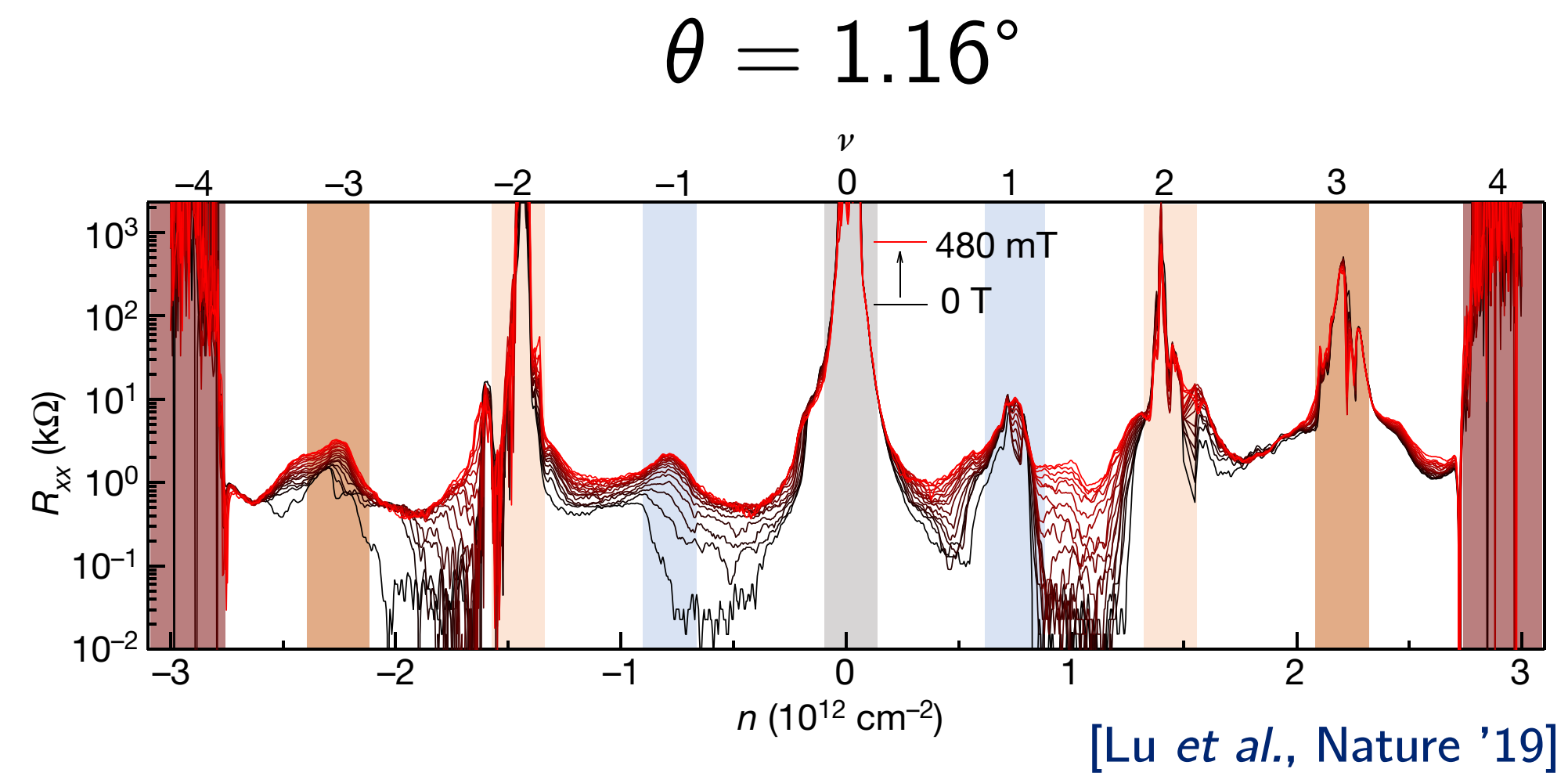
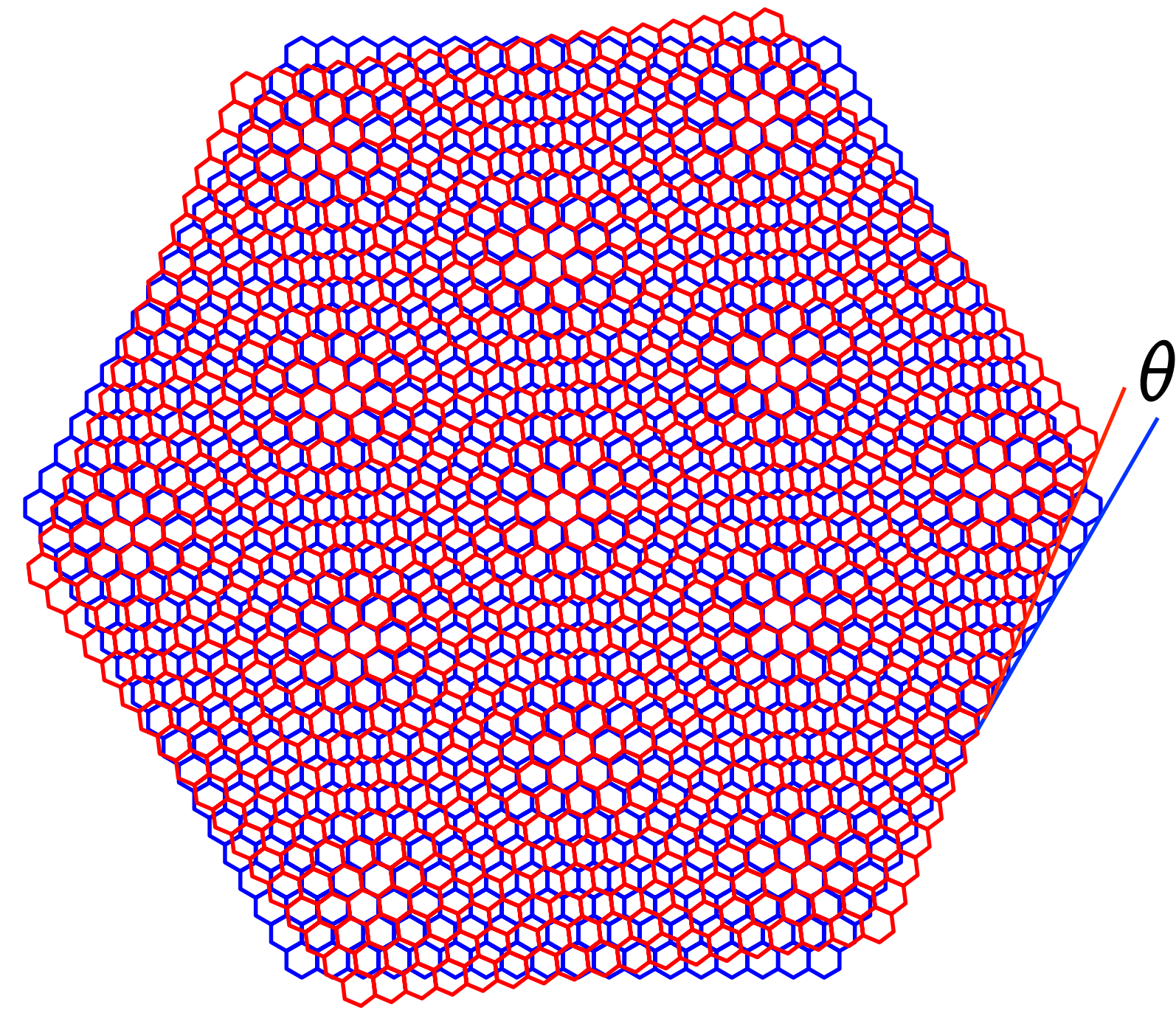
Twisted bilayer graphene



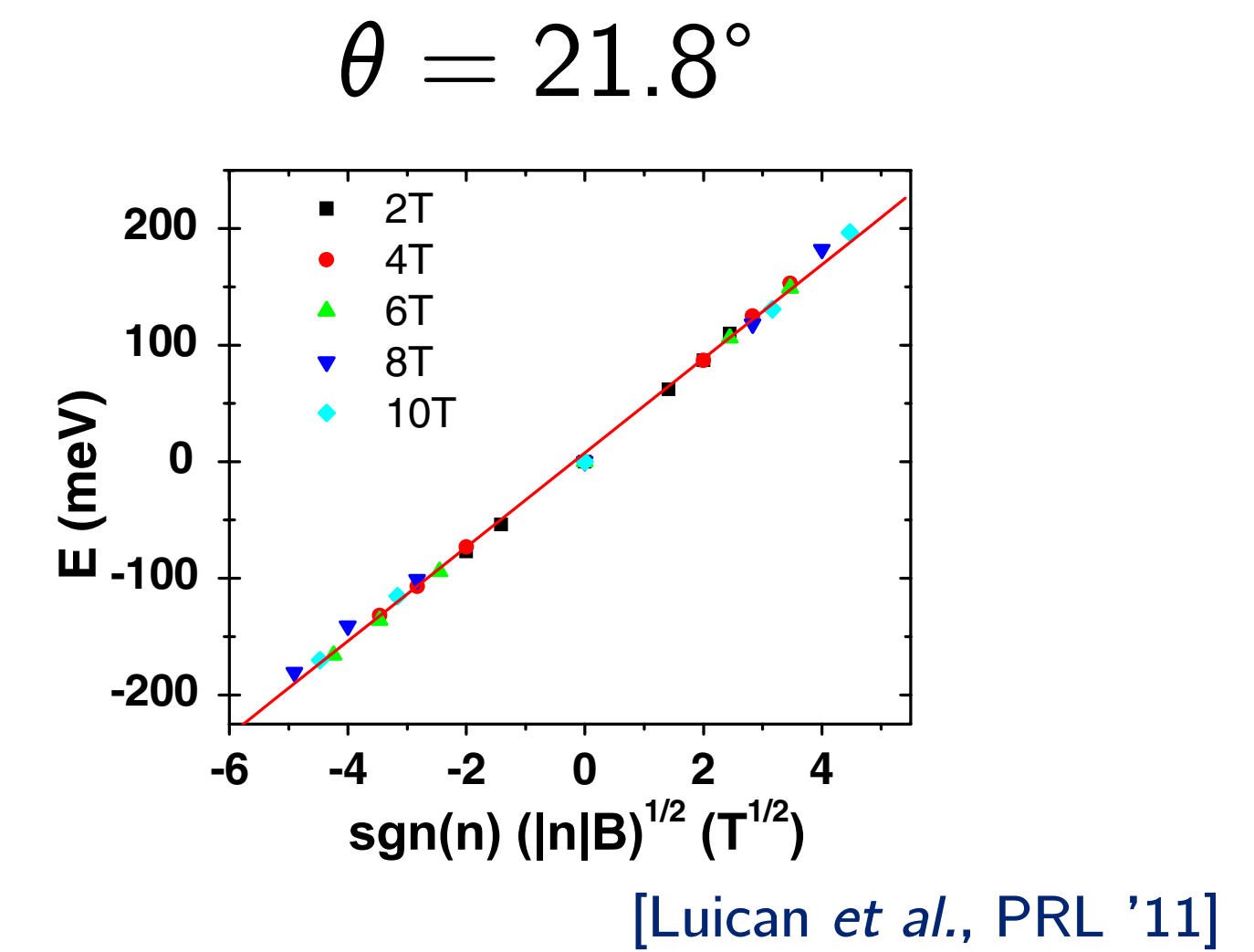
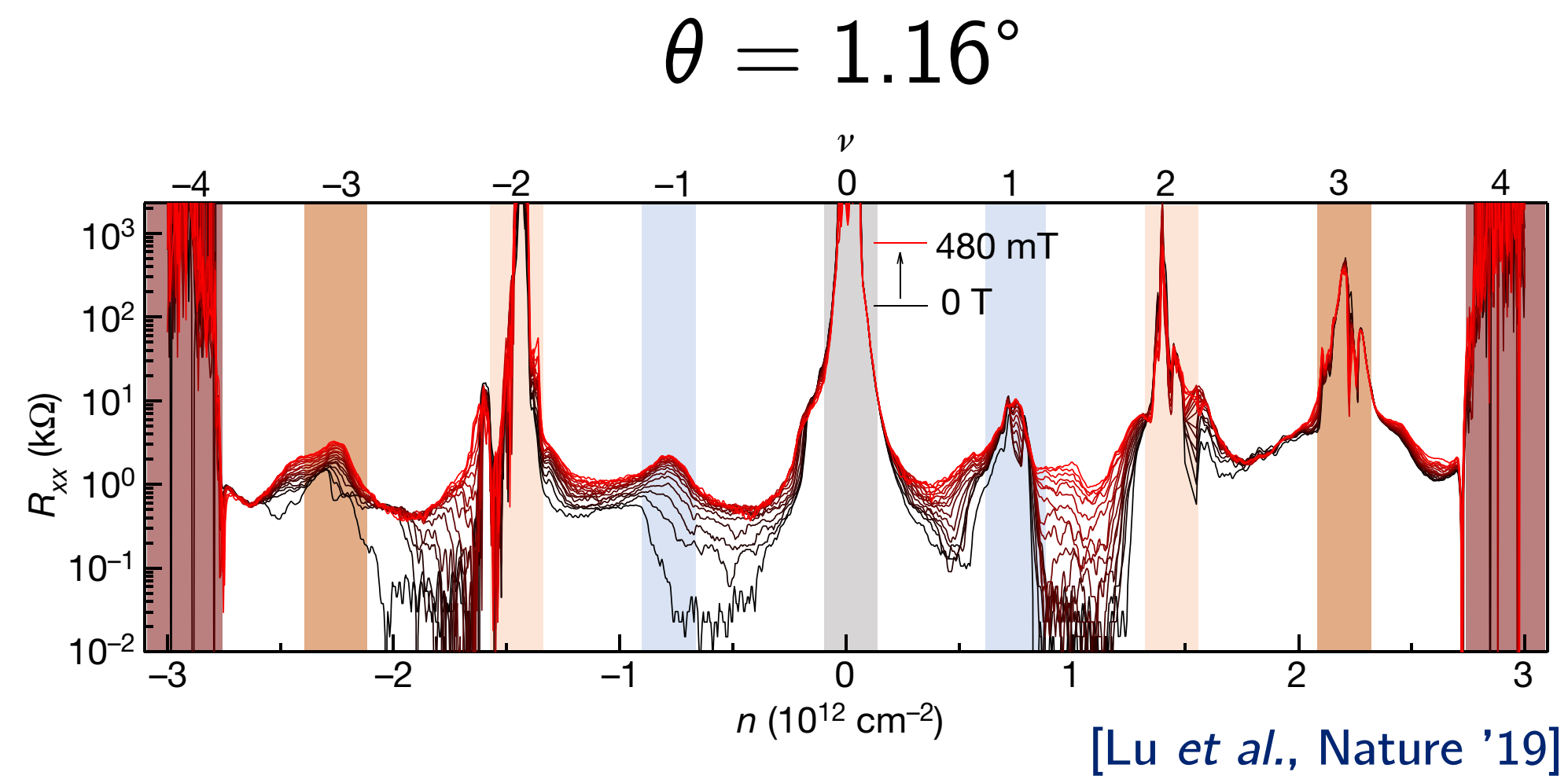
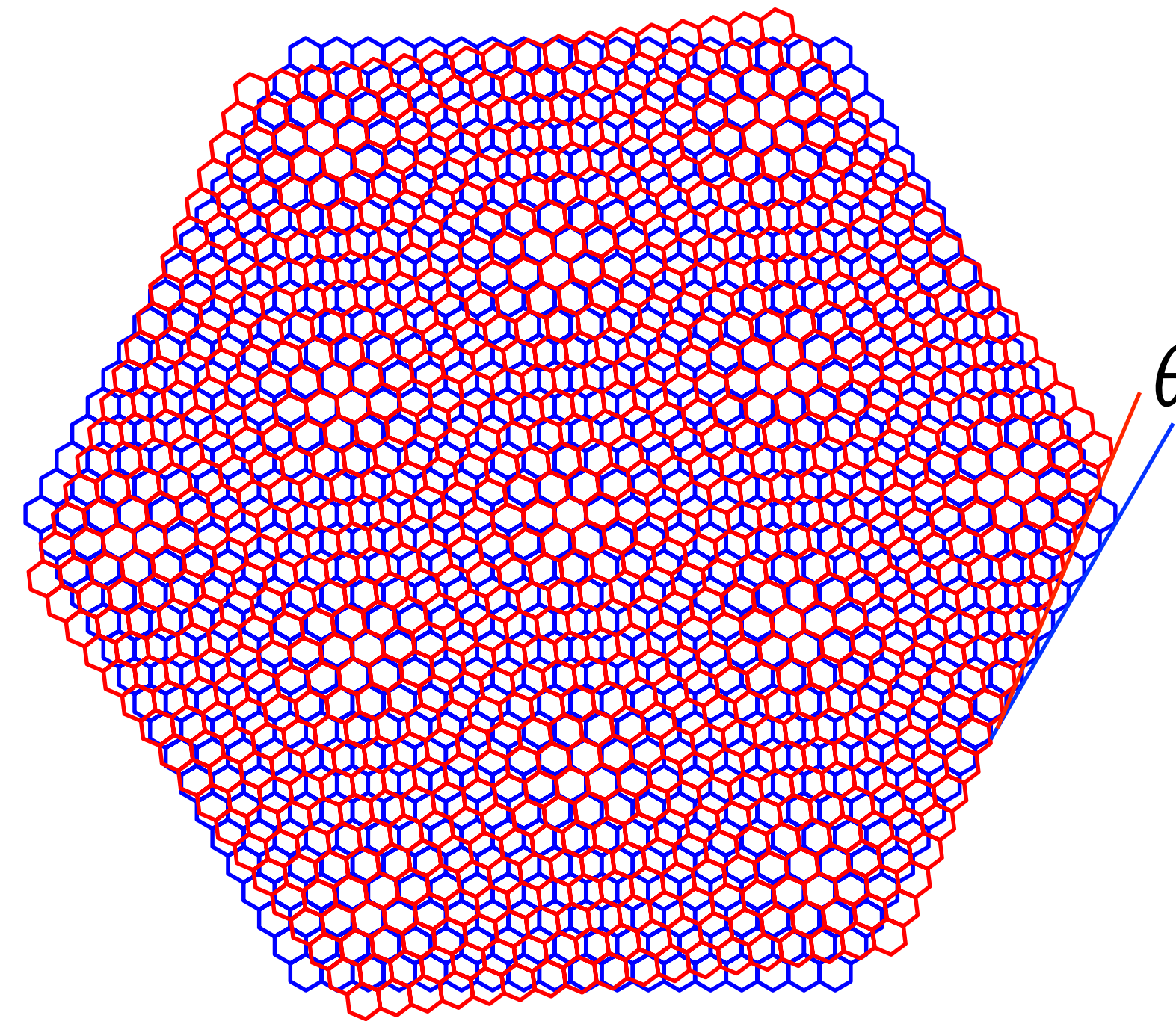
Twisted bilayer graphene



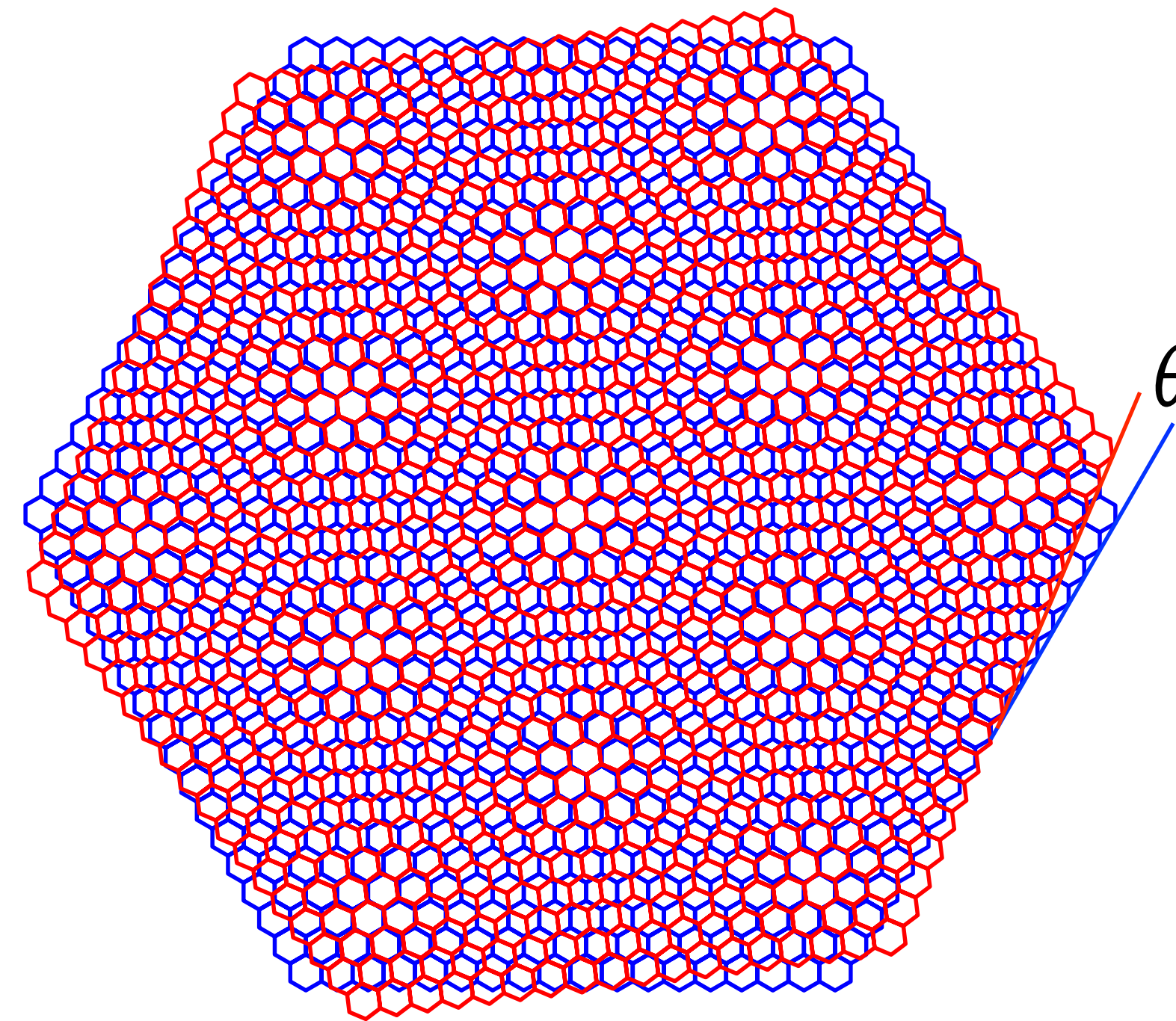
Twisted bilayer graphene



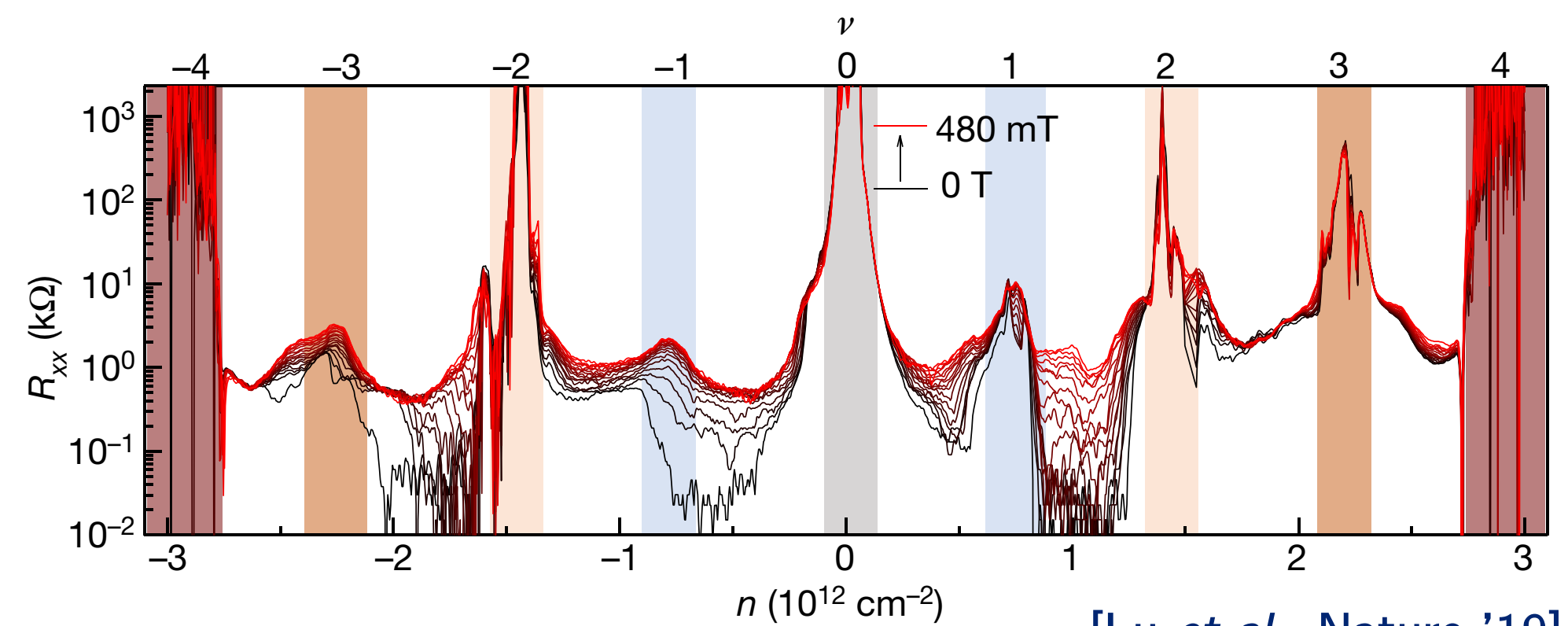
Twisted bilayer graphene



Twisted bilayer graphene

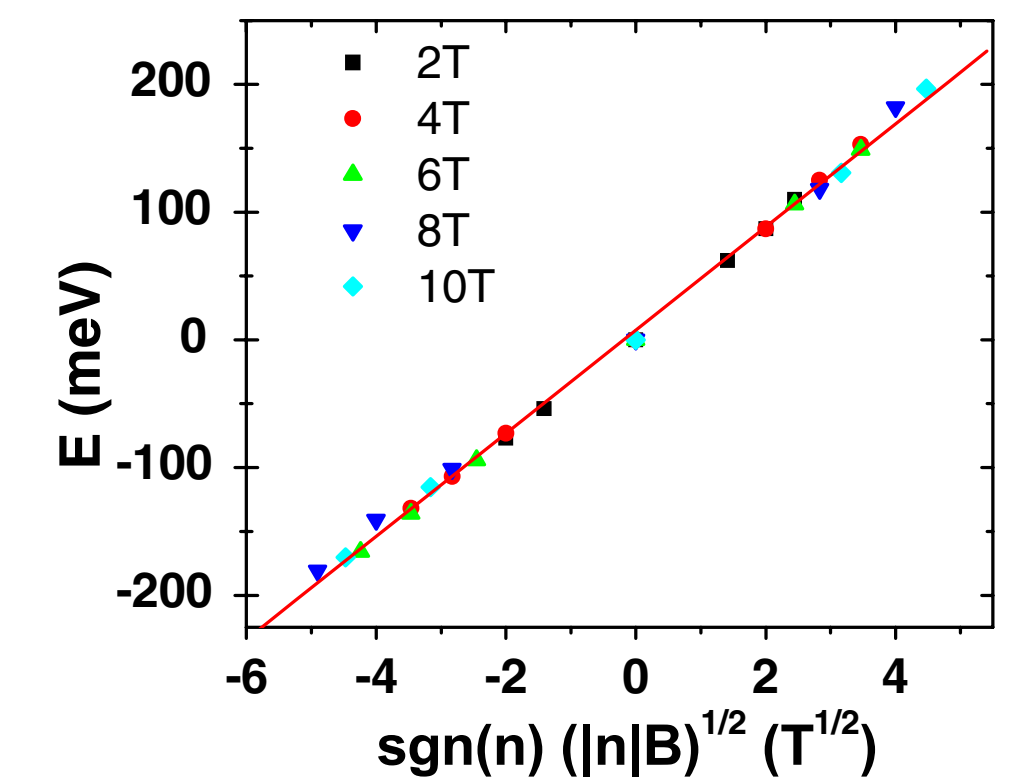


$$\theta = 1.16^\circ$$

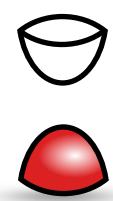


[Lu *et al.*, Nature '19]

$$\theta = 21.8^\circ$$



[Luican *et al.*, PRL '11]



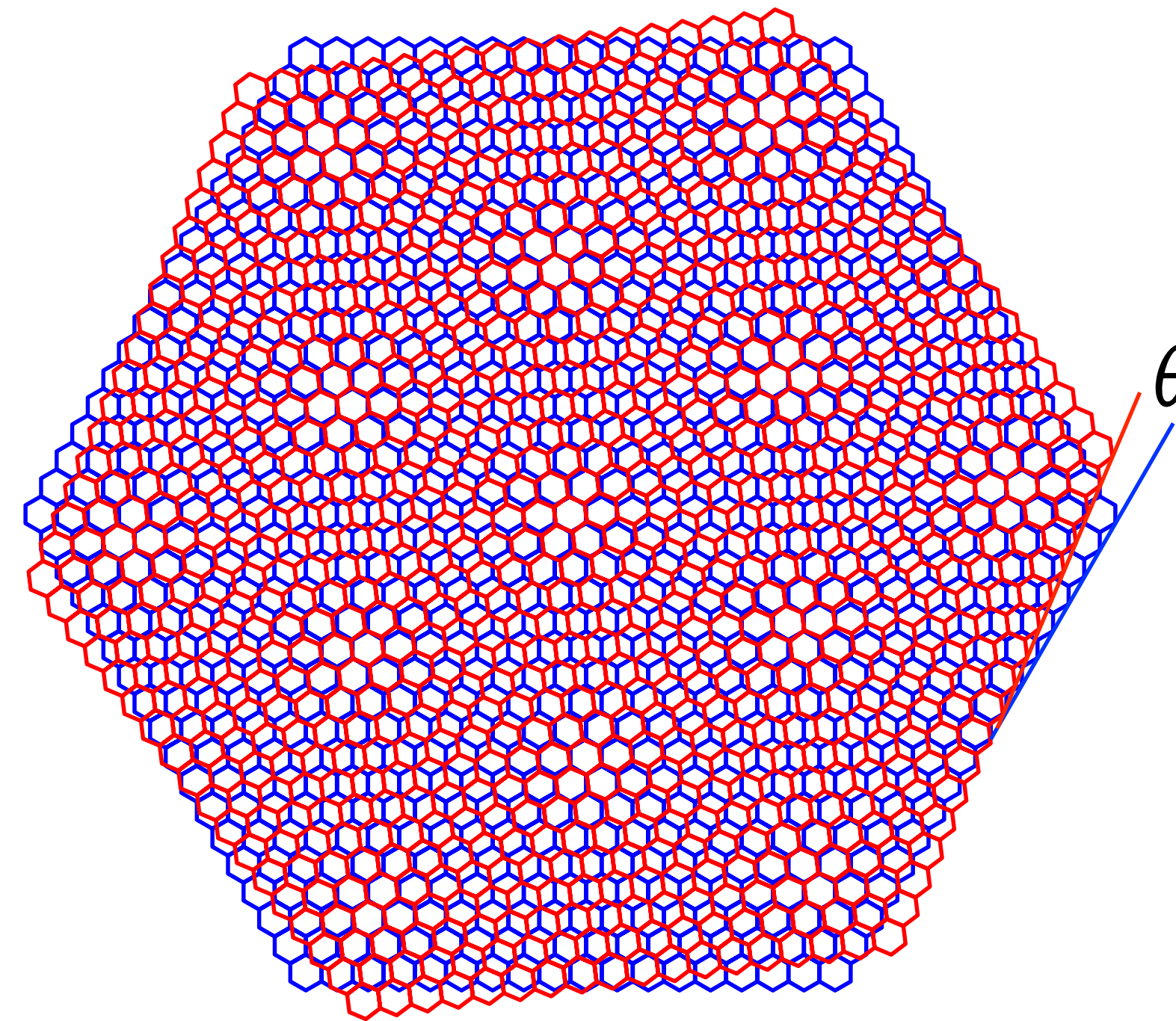
Correlated insulator



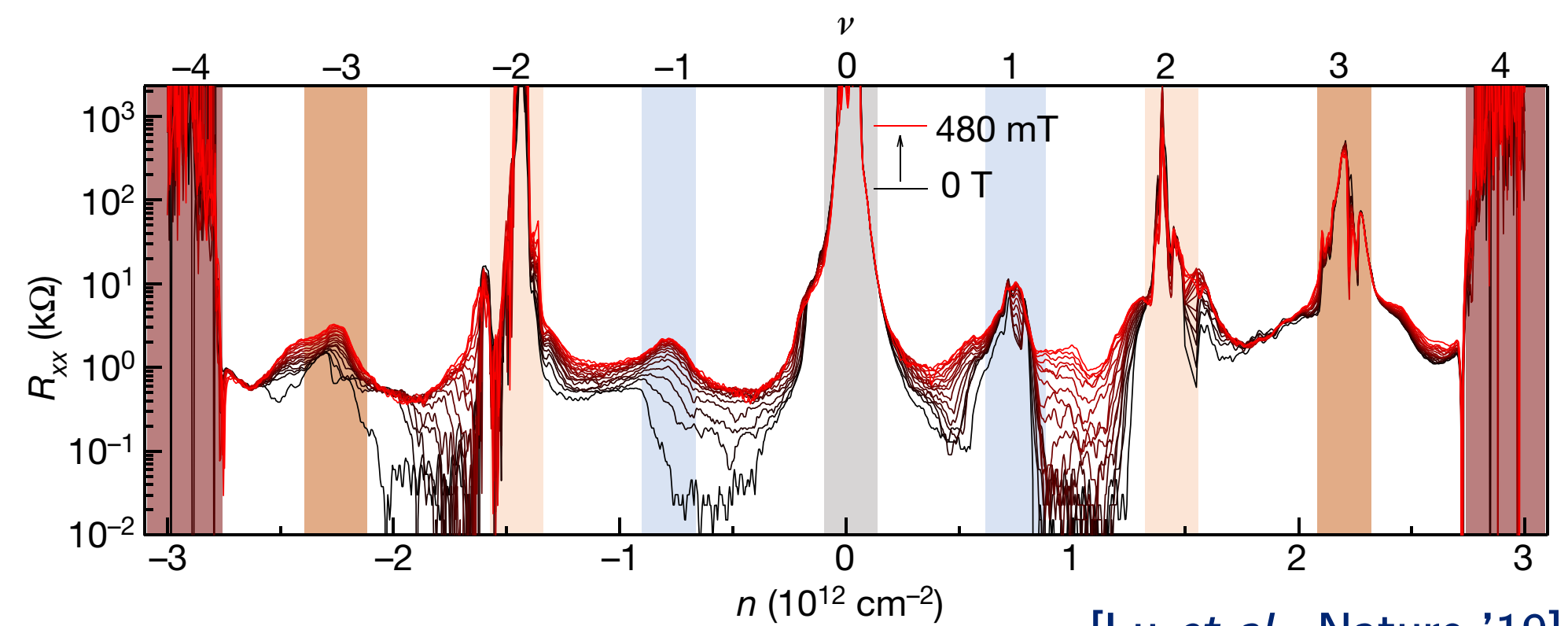
Dirac semimetal

θ

Twisted bilayer graphene

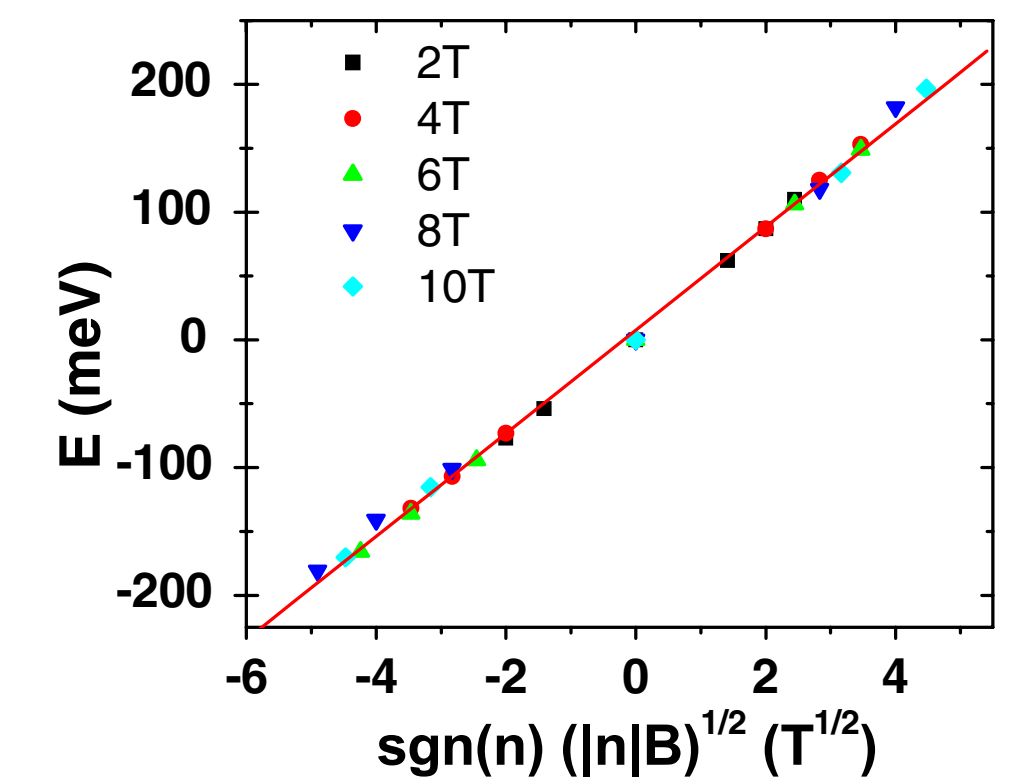


$$\theta = 1.16^\circ$$



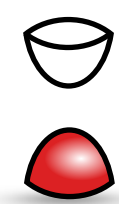
[Lu *et al.*, Nature '19]

$$\theta = 21.8^\circ$$



[Luican *et al.*, PRL '11]

?



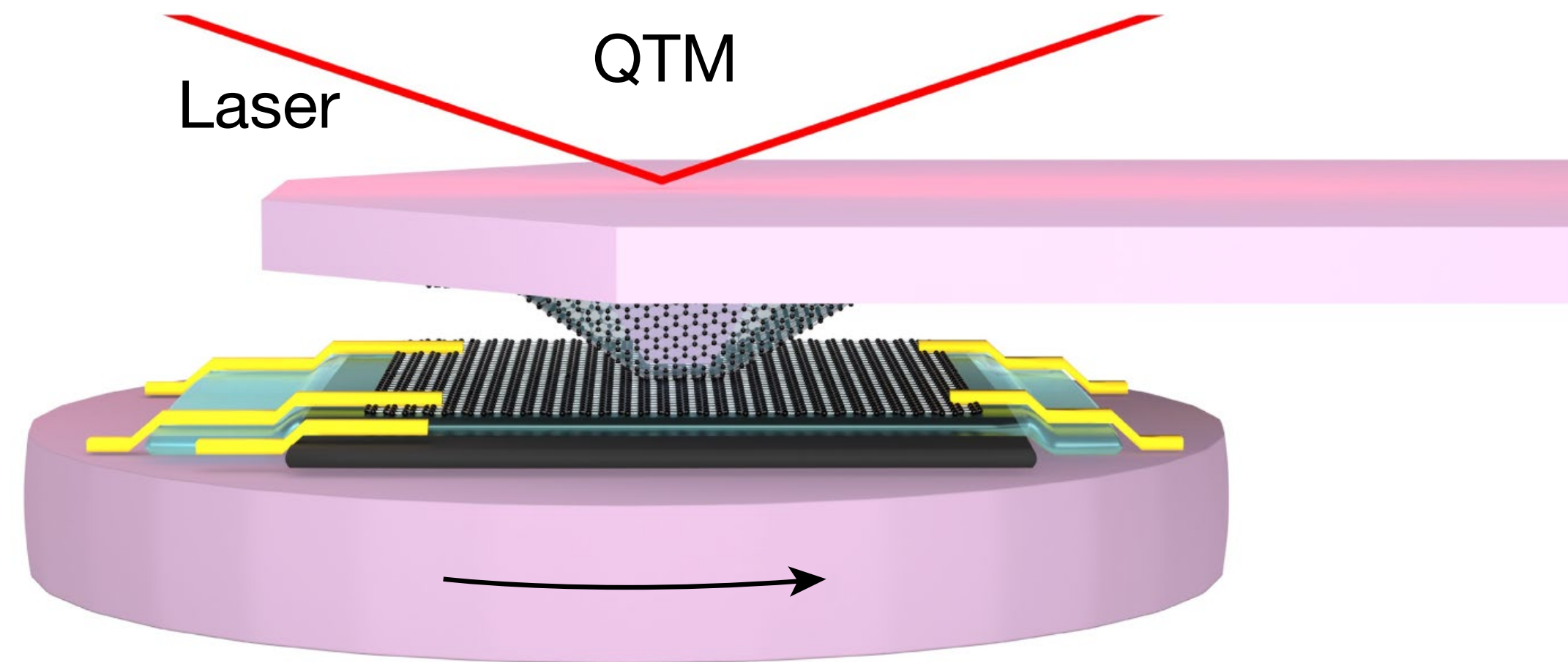
Correlated insulator



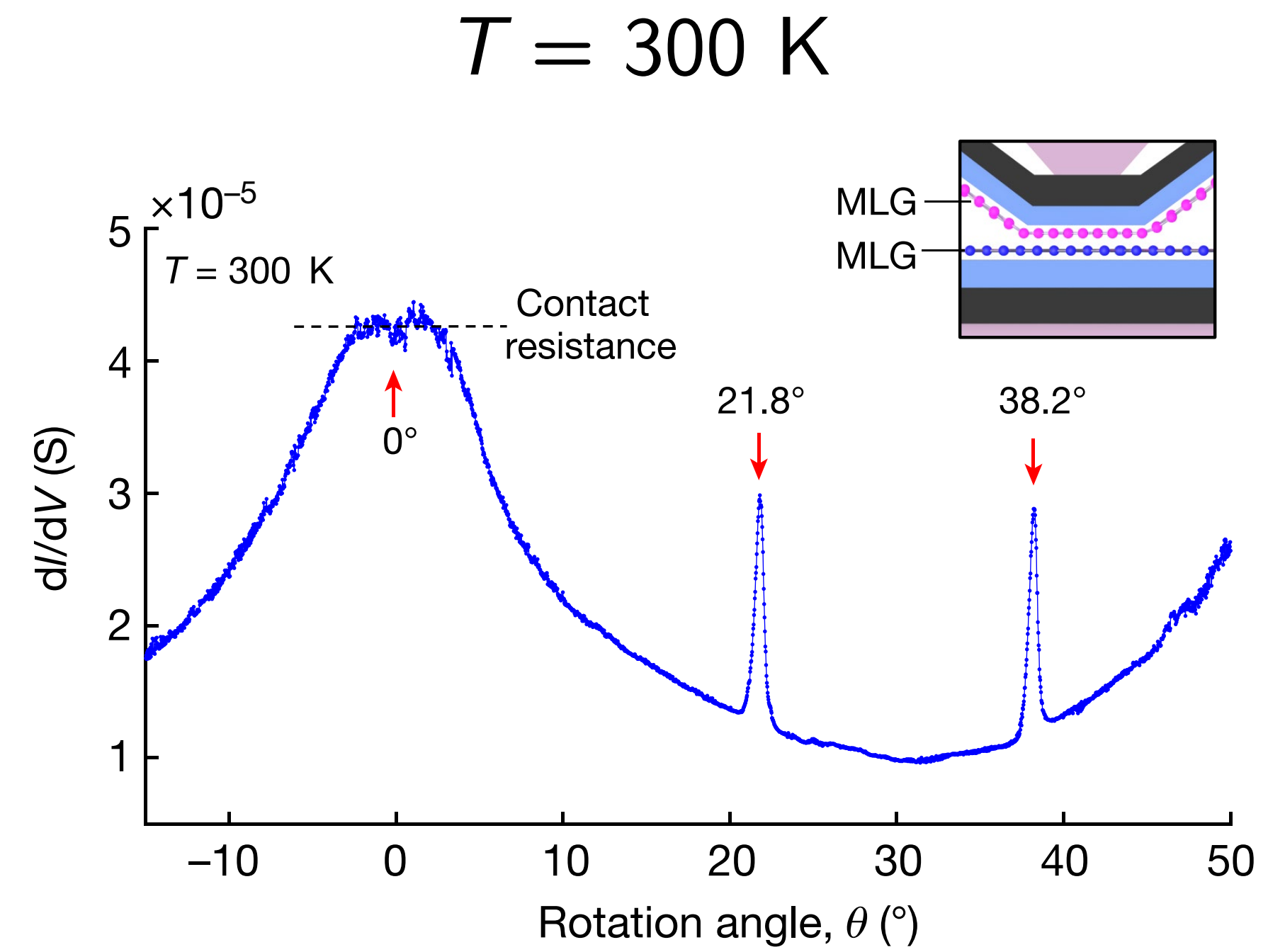
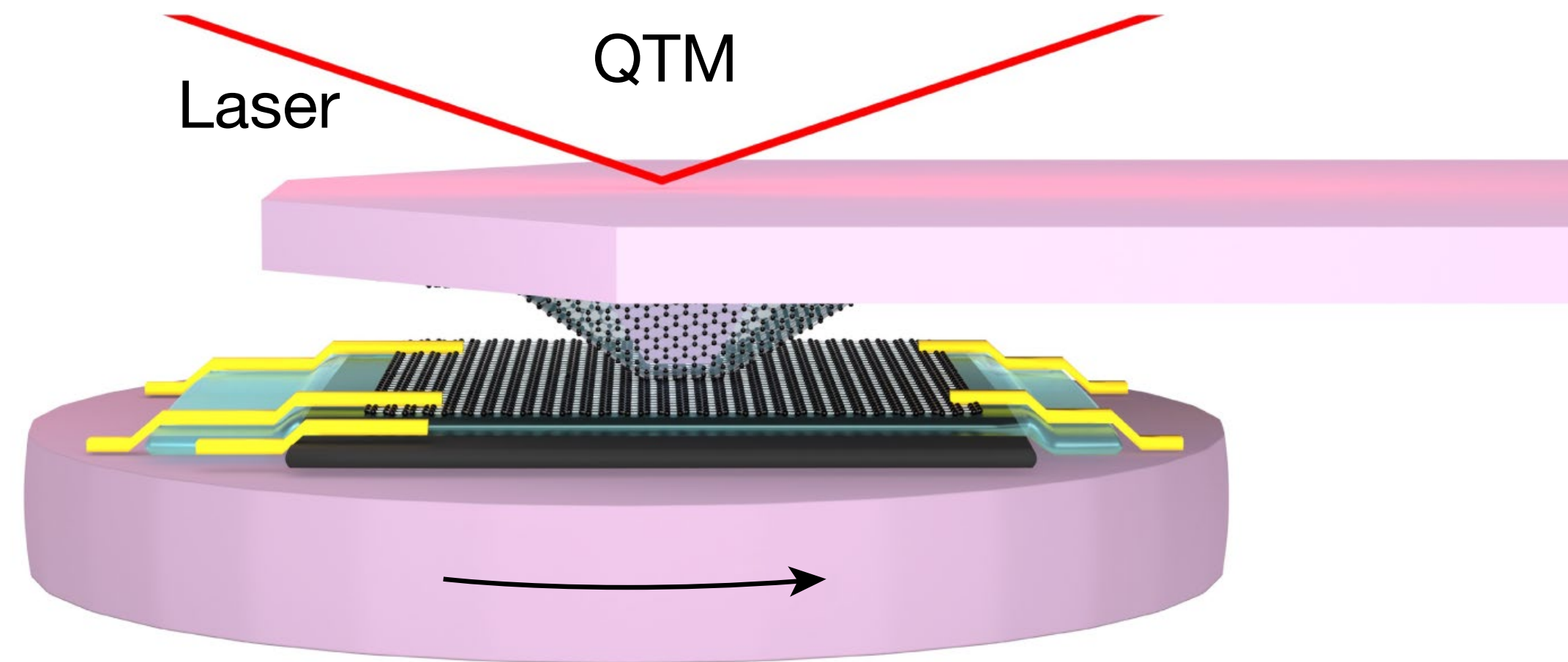
Dirac semimetal

θ

Quantum twisting microscope



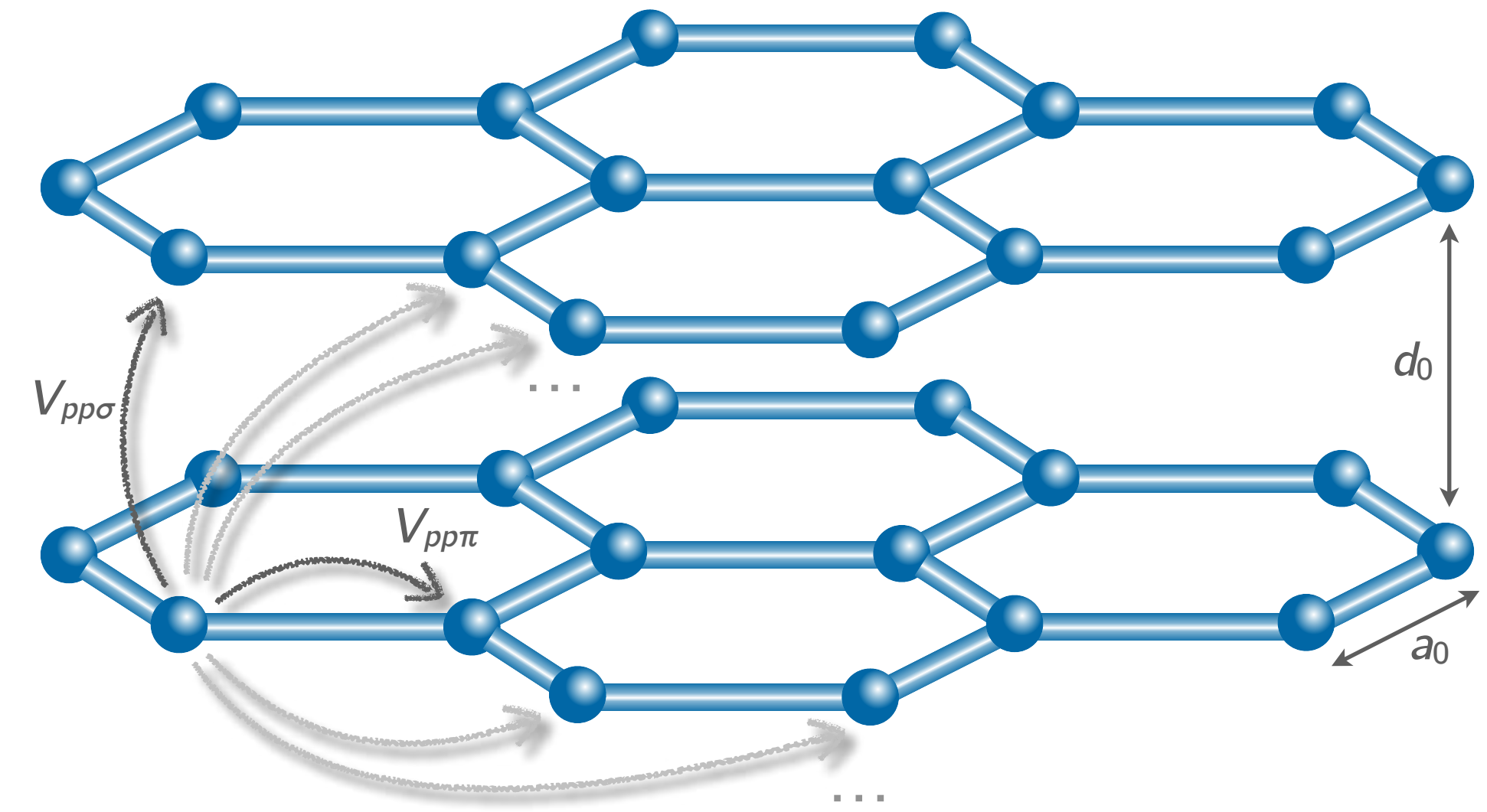
Quantum twisting microscope



Tight-binding model

Hamiltonian:

$$\mathcal{H} = \sum_{i \neq j} t(\mathbf{R}_i - \mathbf{R}_j) c_i^\dagger c_j$$



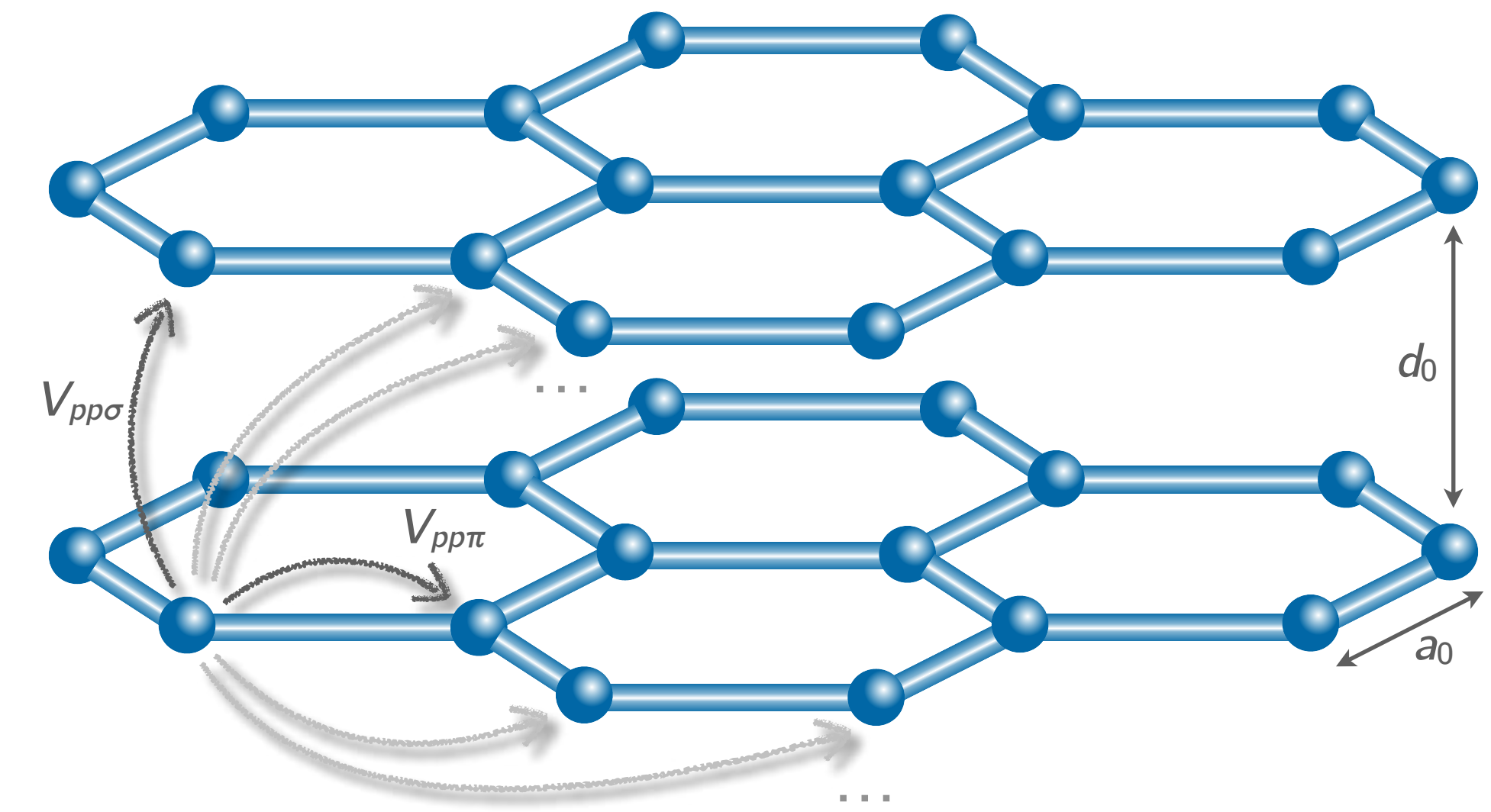
Tight-binding model

Hamiltonian:

$$\mathcal{H} = \sum_{i \neq j} t(\mathbf{R}_i - \mathbf{R}_j) c_i^\dagger c_j$$

Slater-Koster hopping:

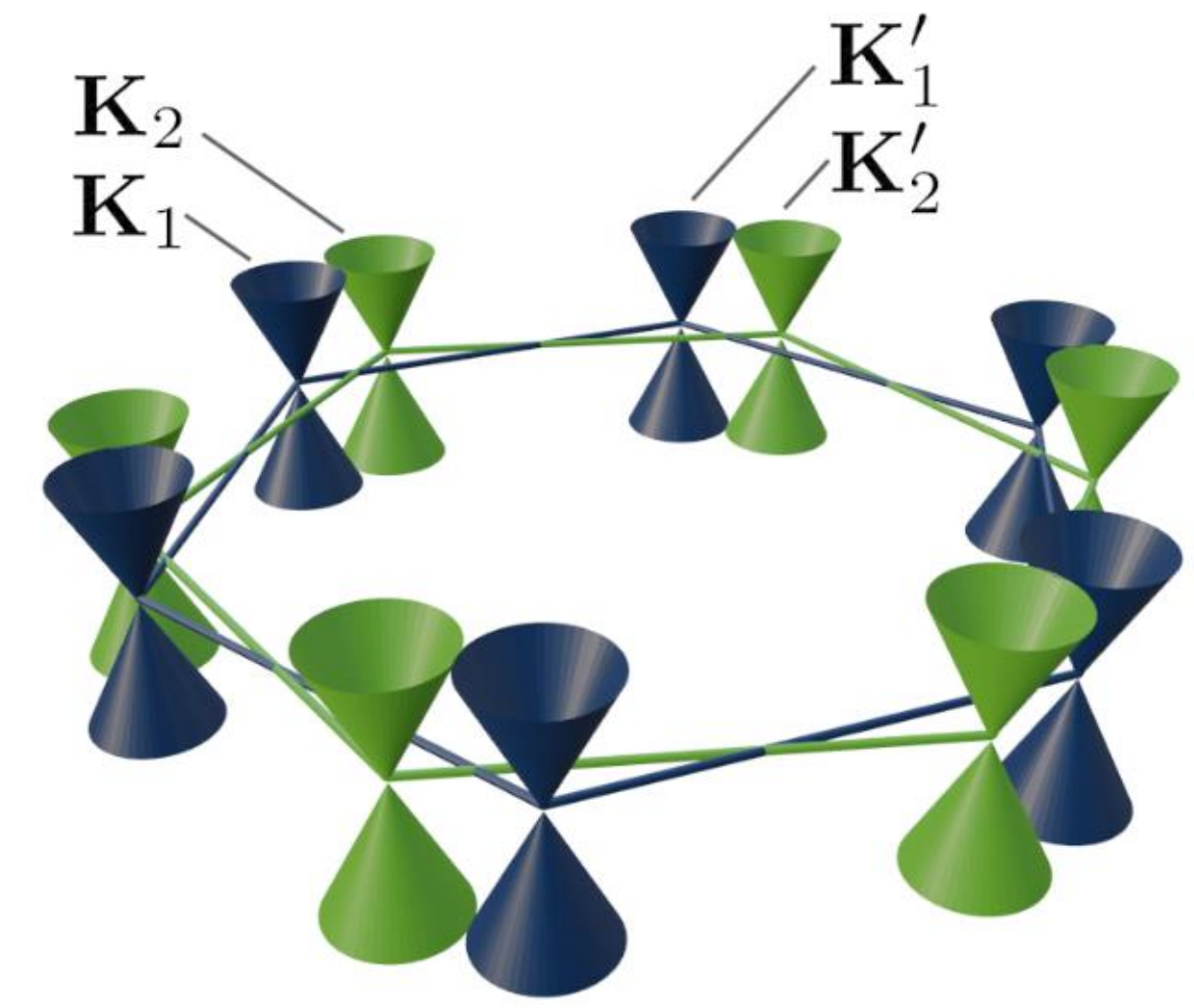
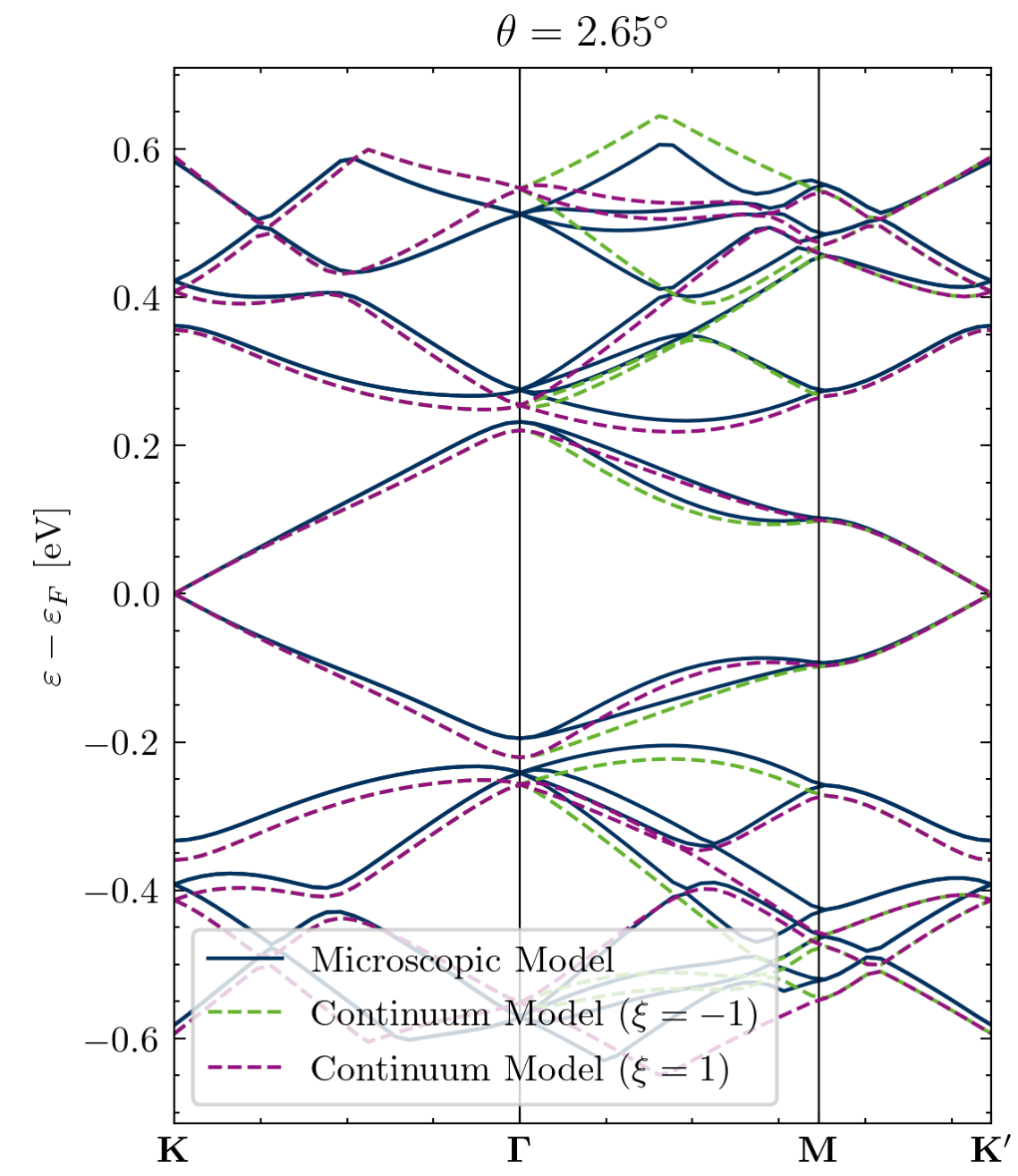
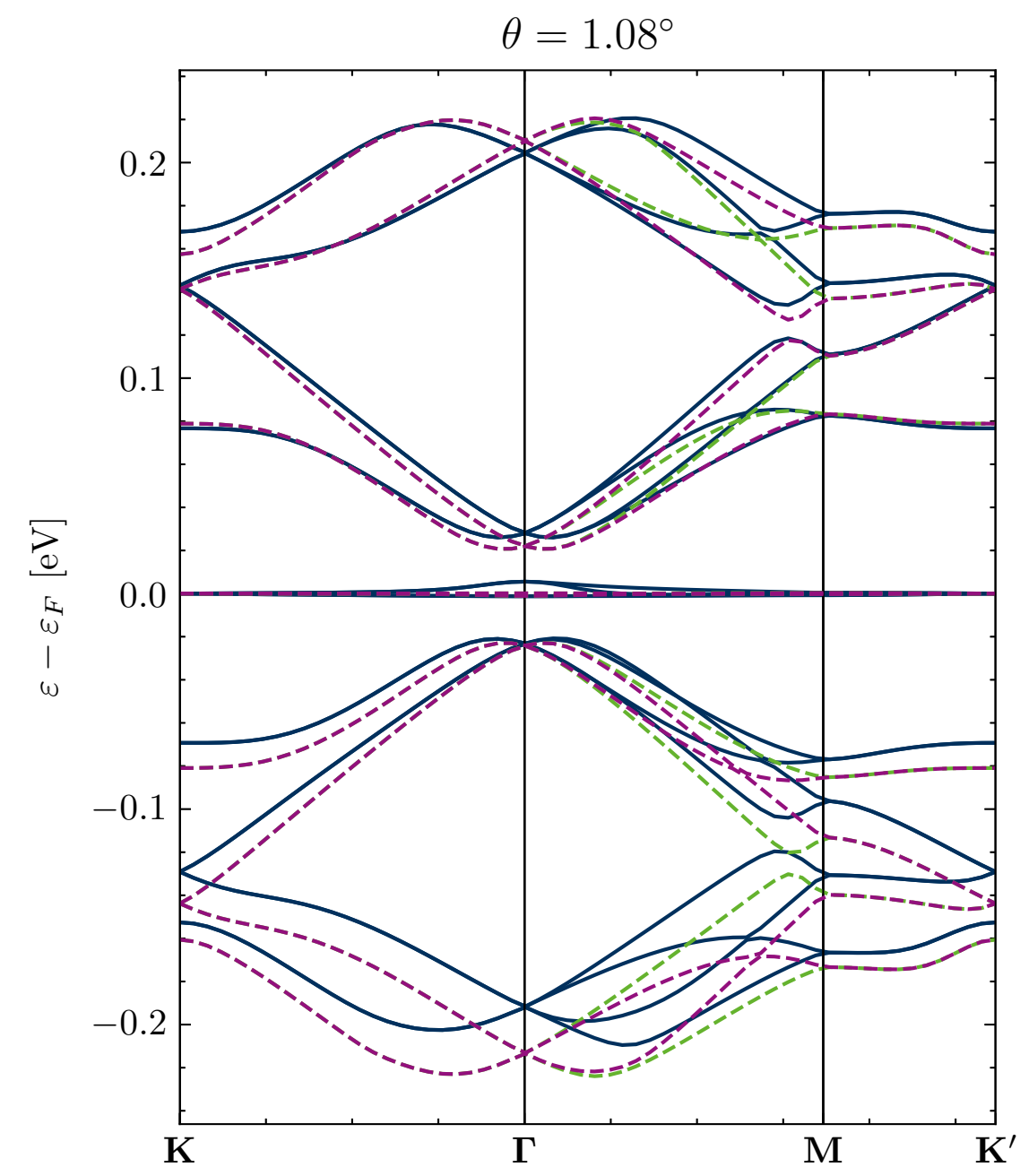
$$t(\mathbf{r}) = \begin{cases} -V_{pp\pi} \frac{x^2 + y^2}{r^2} e^{-\frac{r-a_0}{r_0}} - V_{pp\sigma} \frac{z^2}{r^2} e^{-\frac{r-d_0}{r_0}} & \text{for } a_0 \leq r \leq 6a_0 \\ 0 & \text{for } r > 6a_0 \end{cases}$$



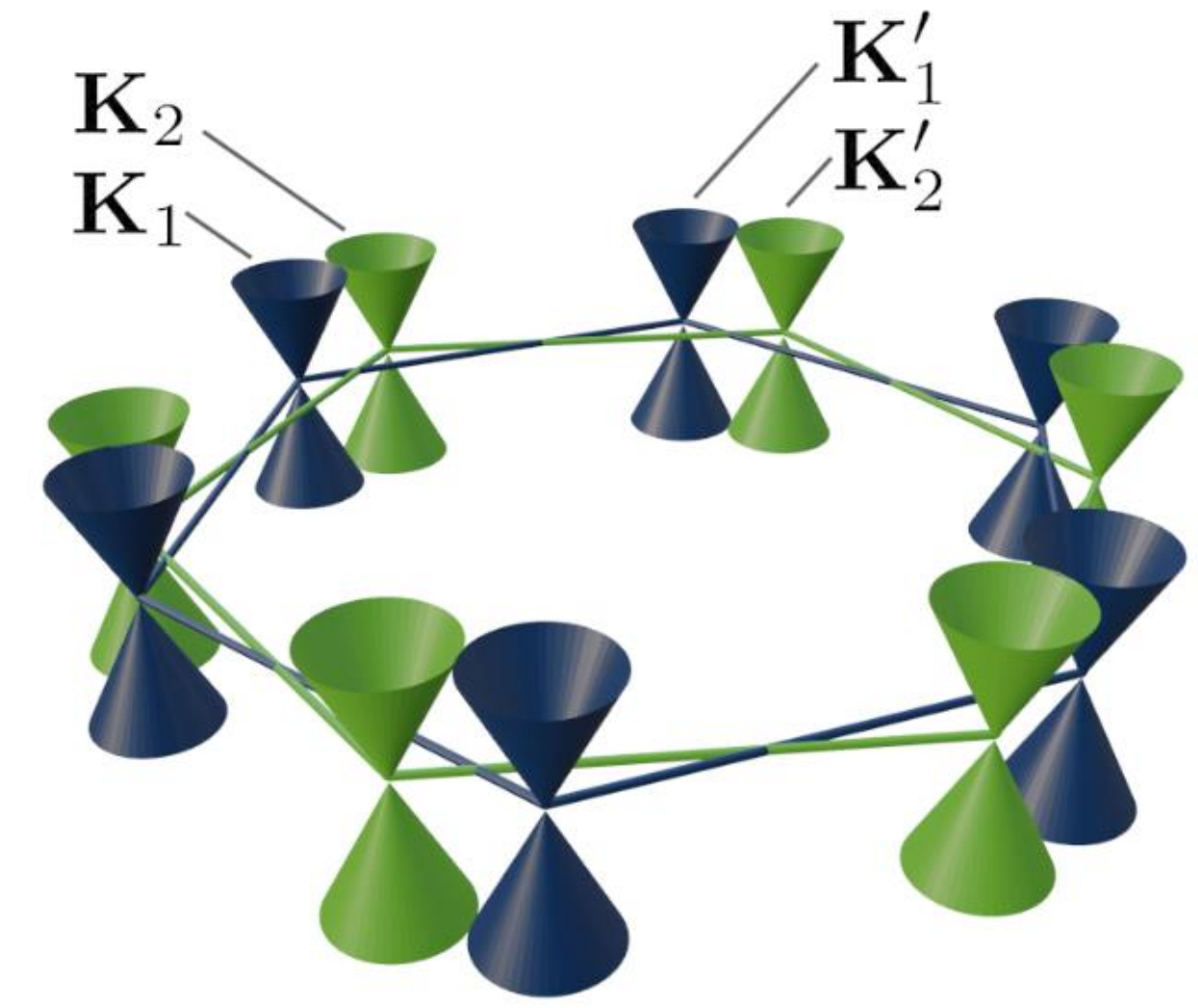
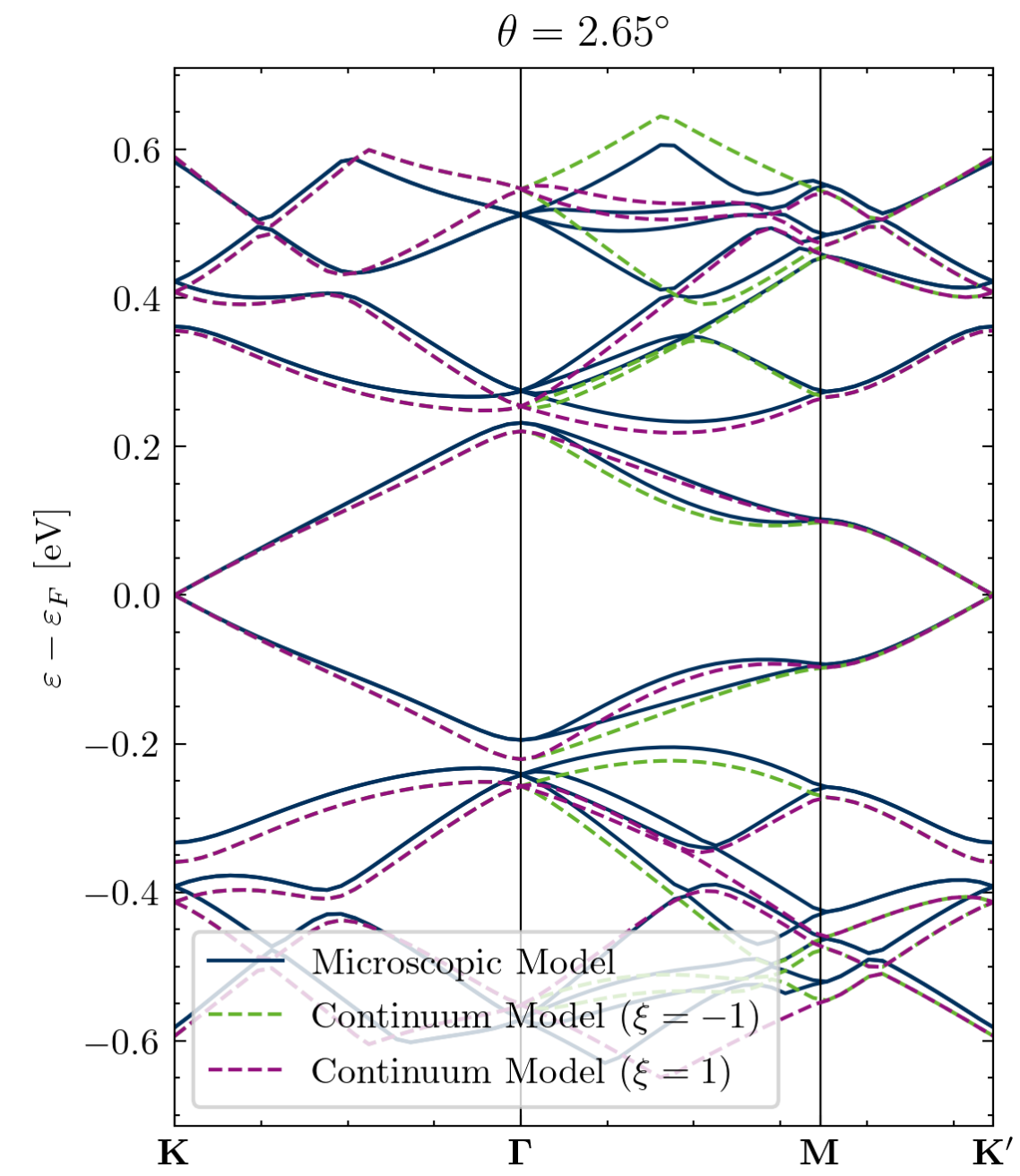
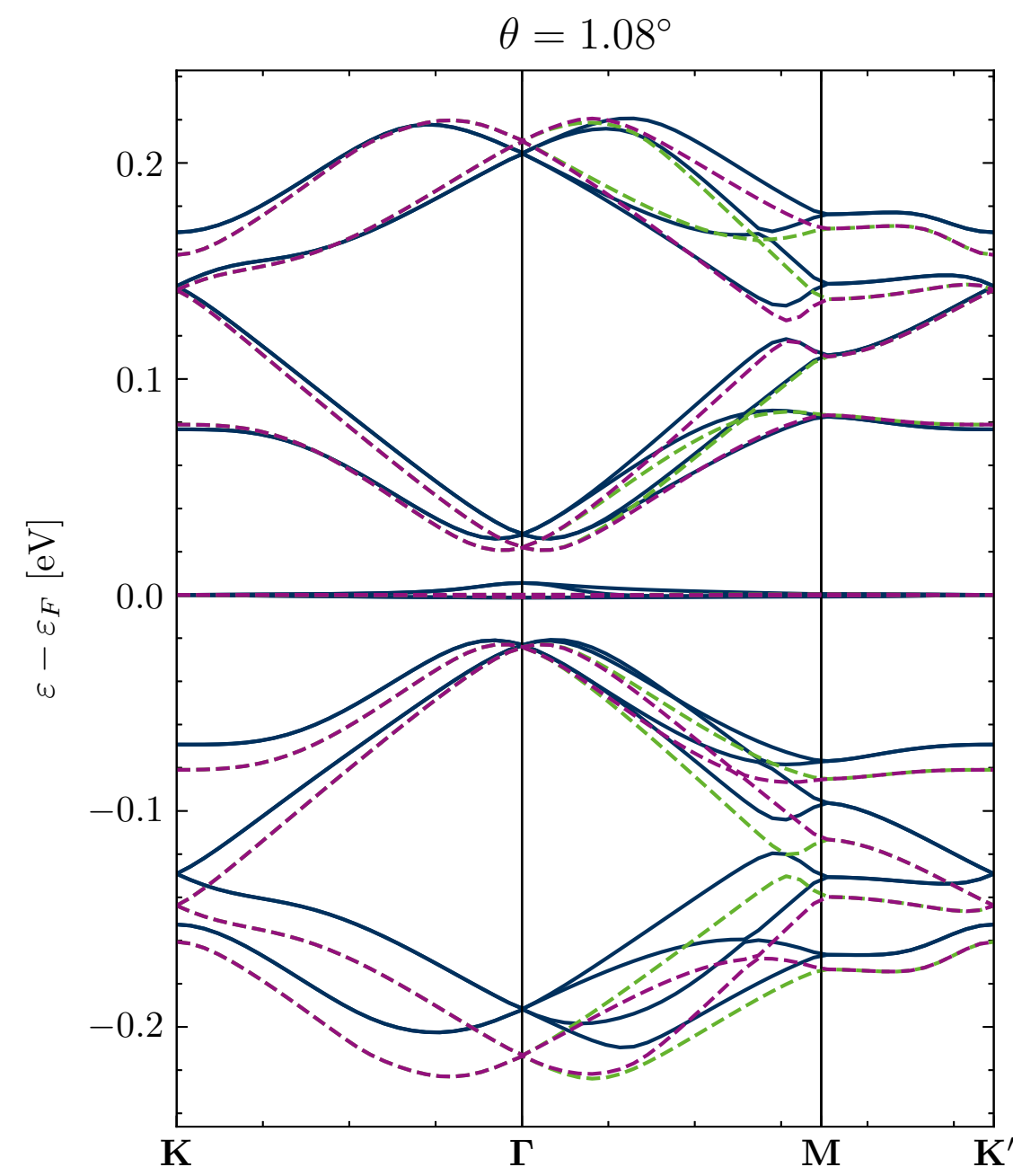
[Moon & Koshino, PRB '13]
[Koshino *et al.*, PRX '18]

... with $V_{pp\pi} \approx -2.7$ eV, $V_{pp\sigma} \approx 0.48$ eV, and decay length $r_0 \approx 0.319a_0$

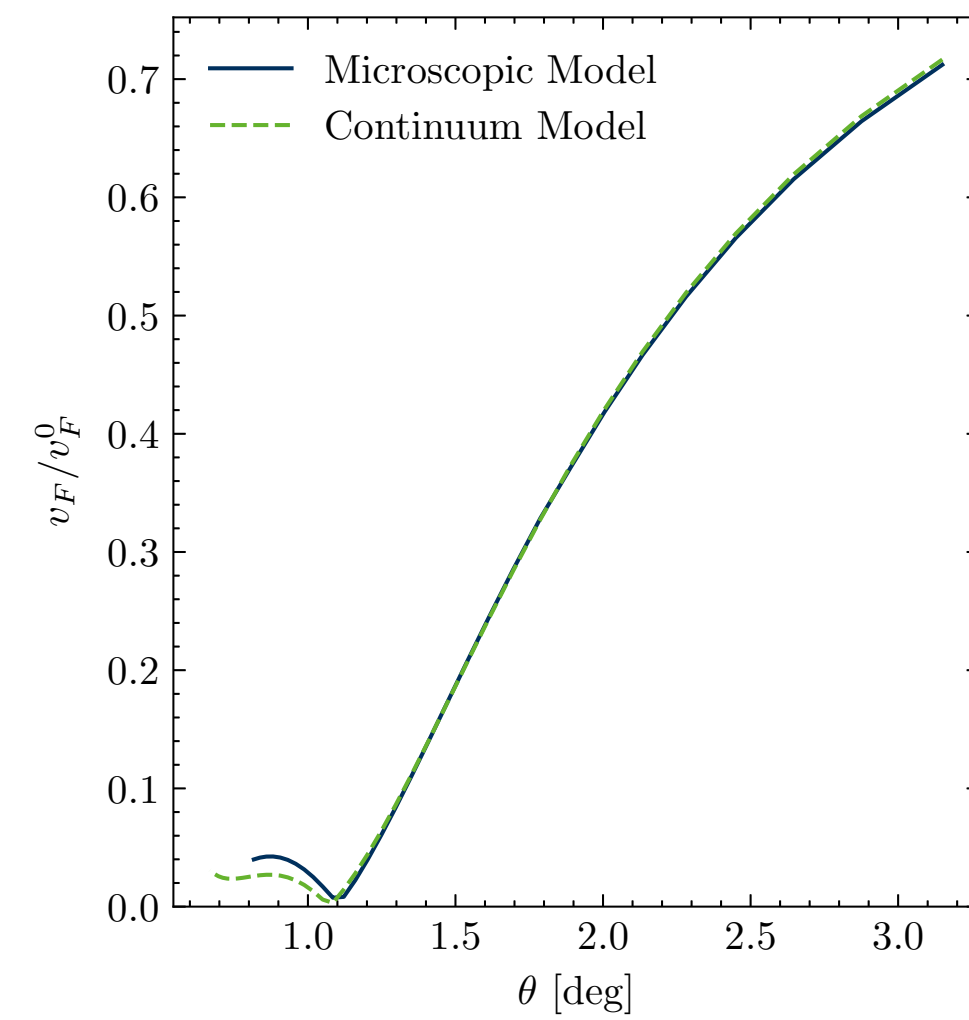
Electronic band structure



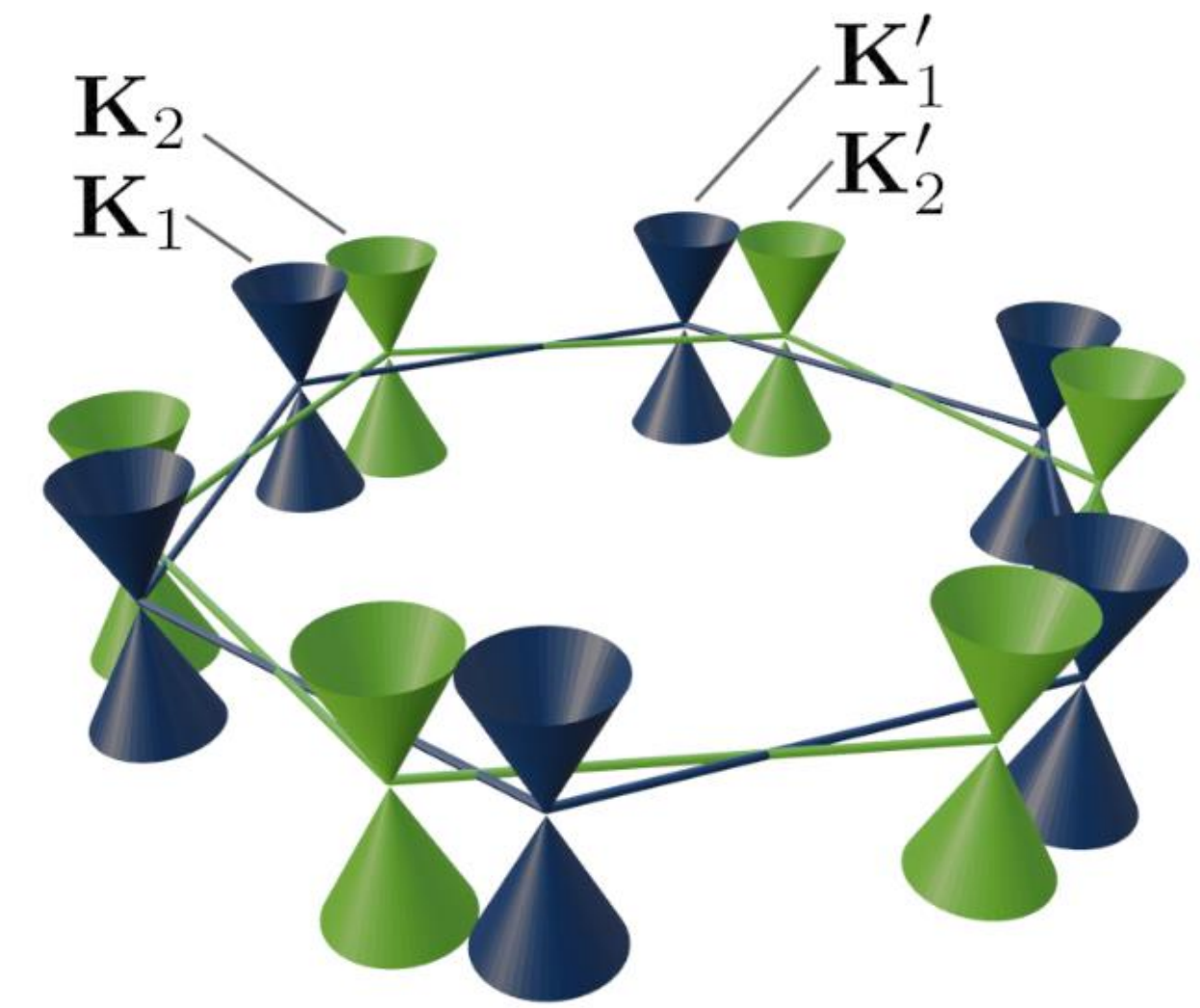
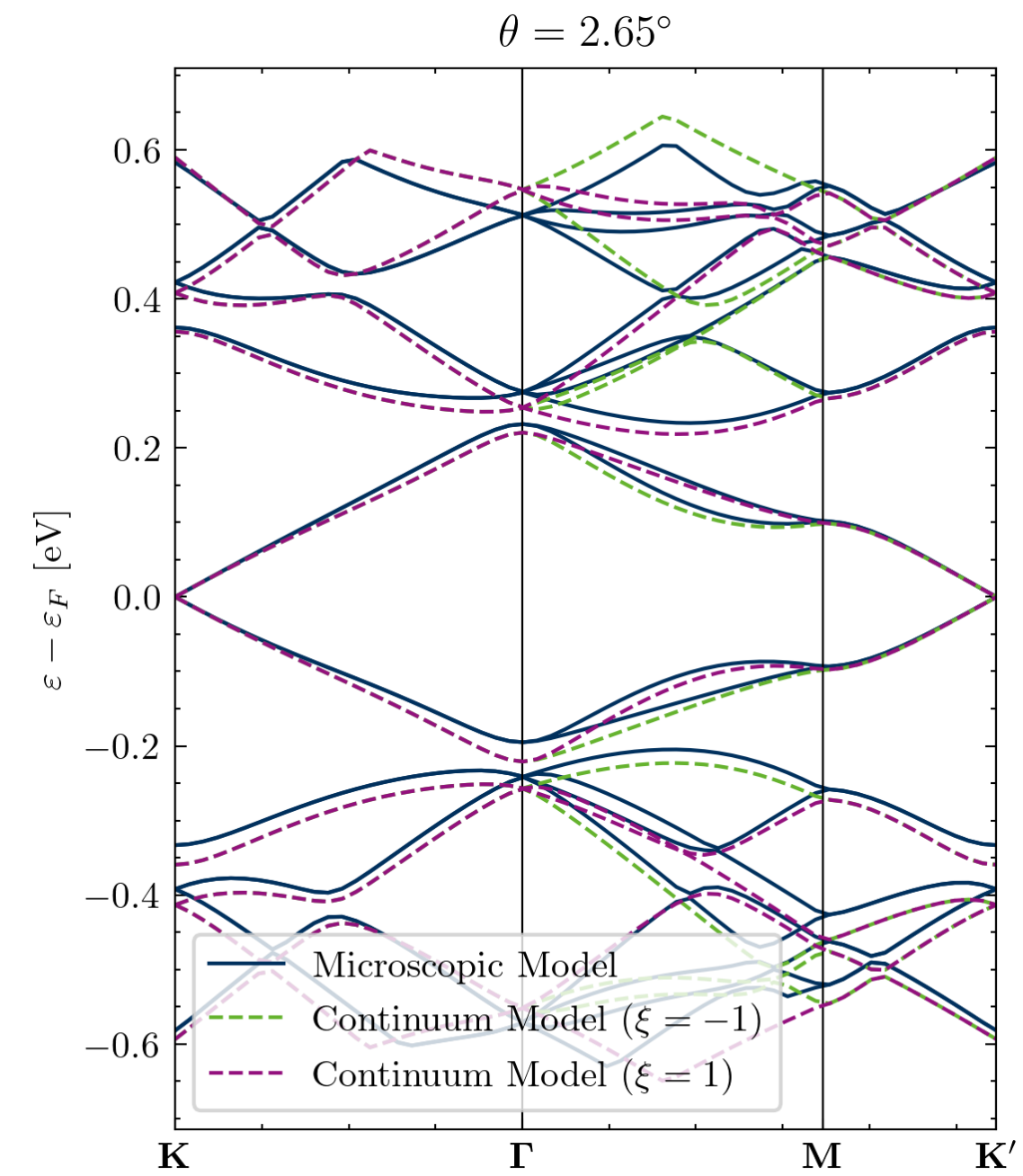
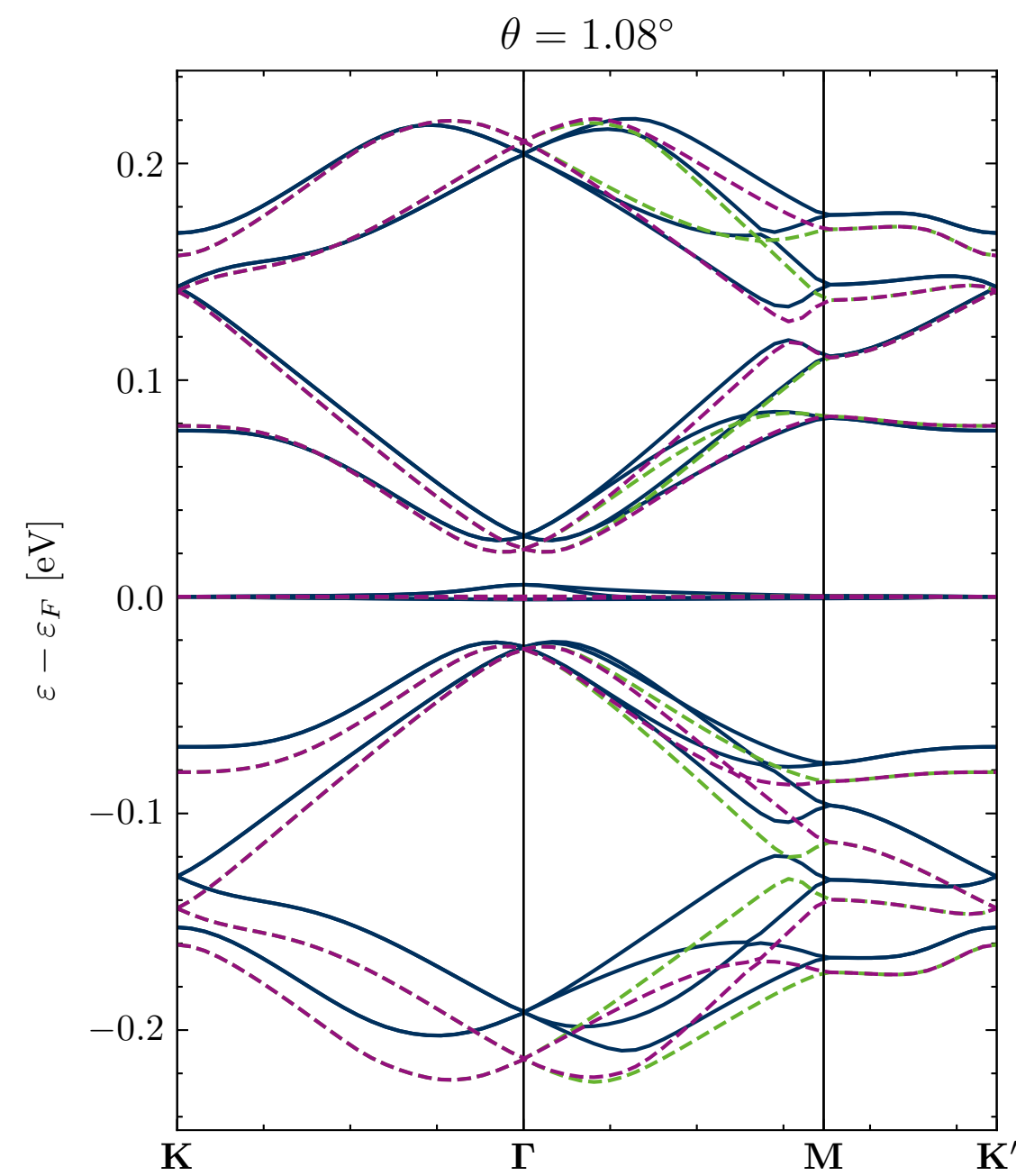
Electronic band structure



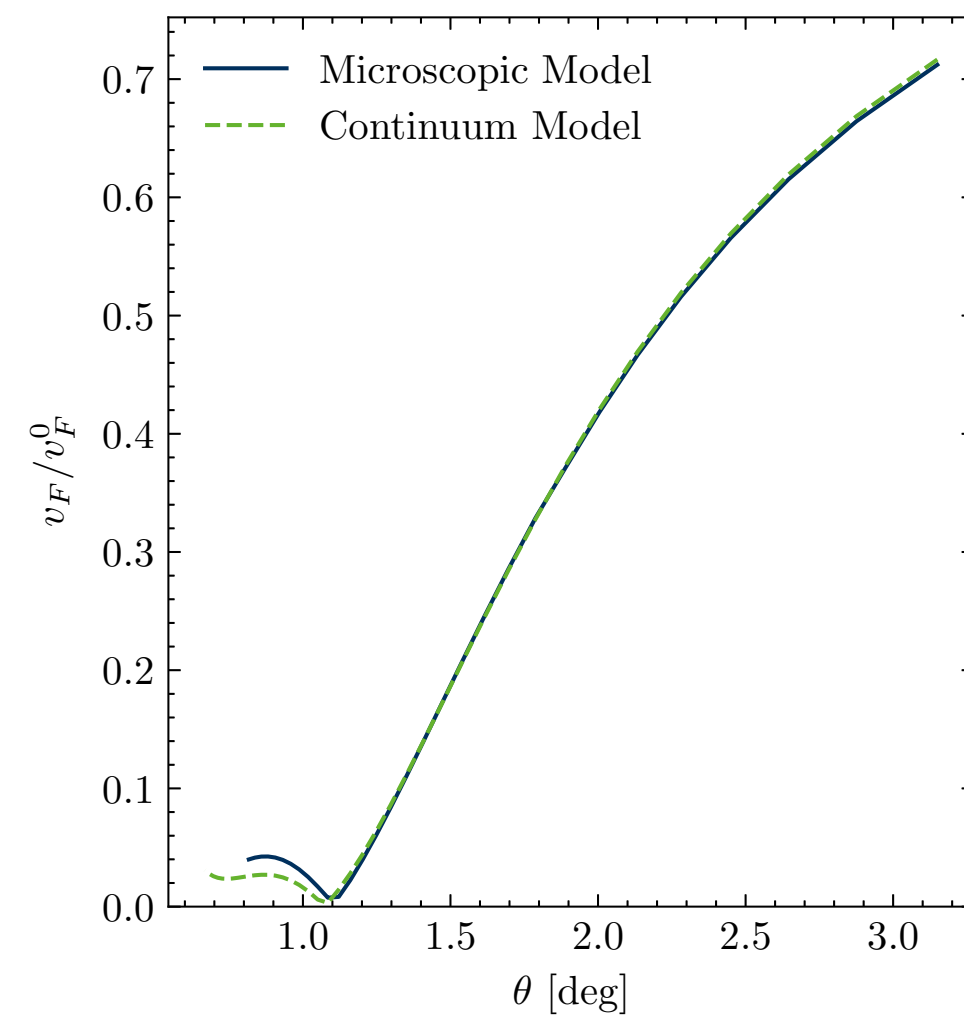
Fermi velocity:



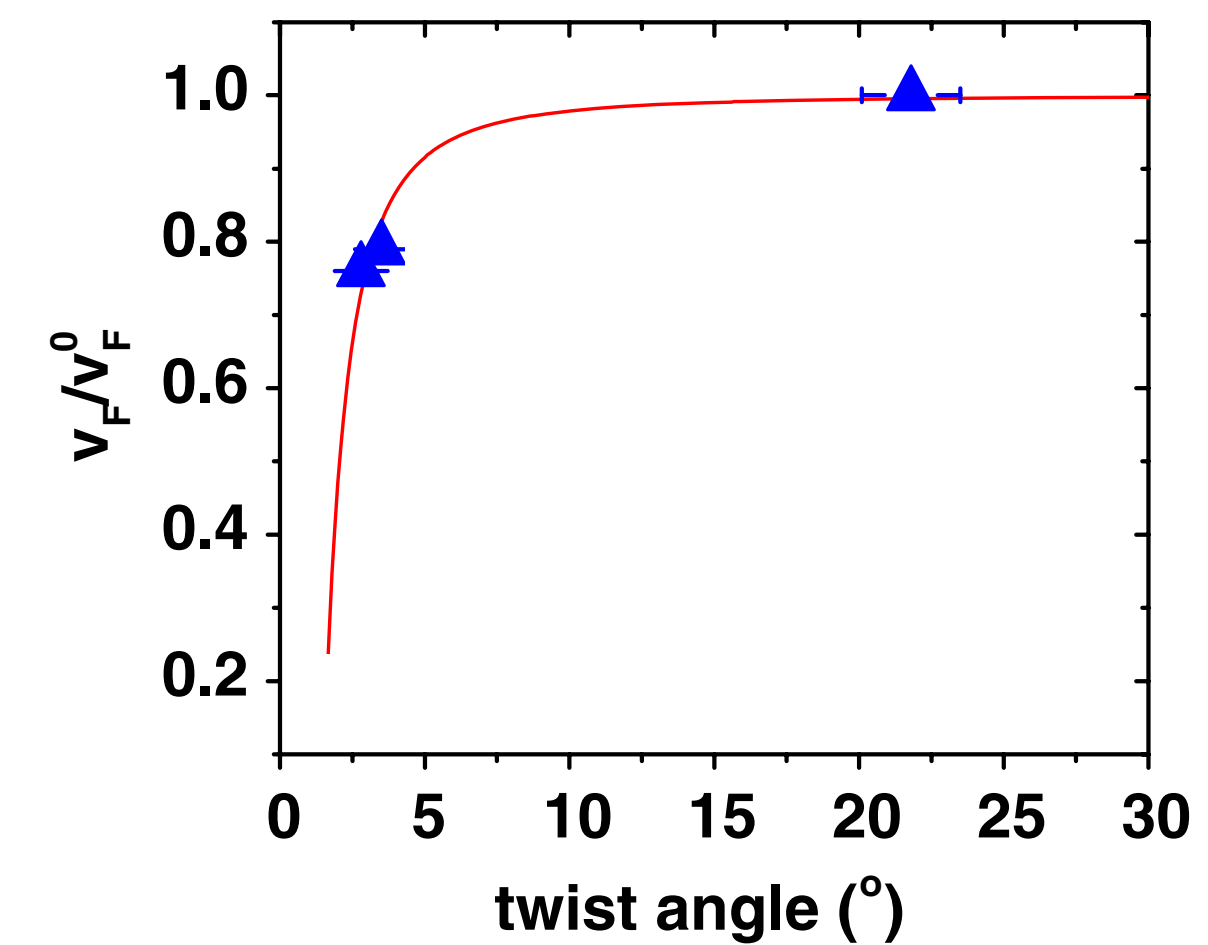
Electronic band structure



Fermi velocity:



Experiment:

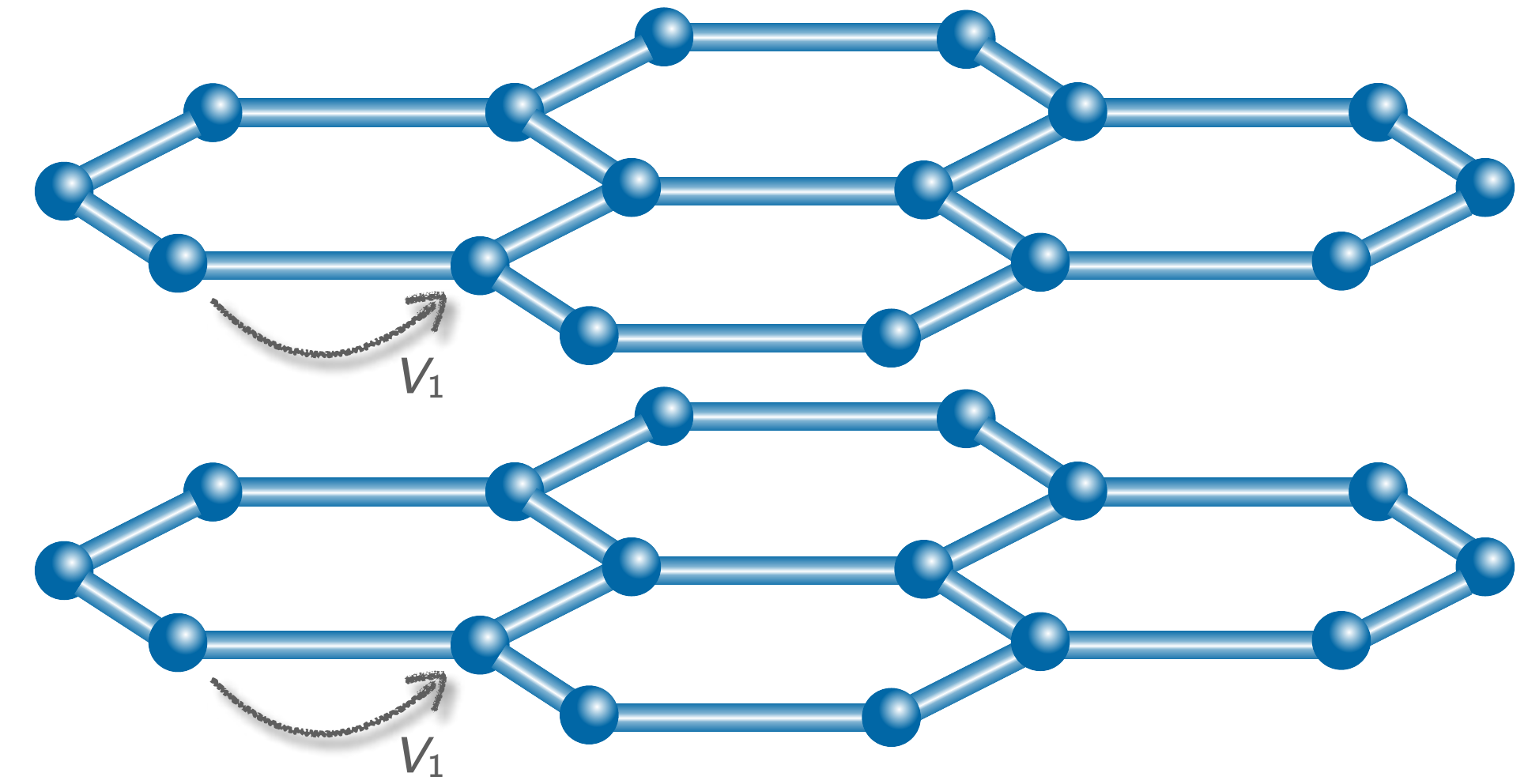


[Luican *et al.*, PRL '11]

Interactions

Toy lattice model:

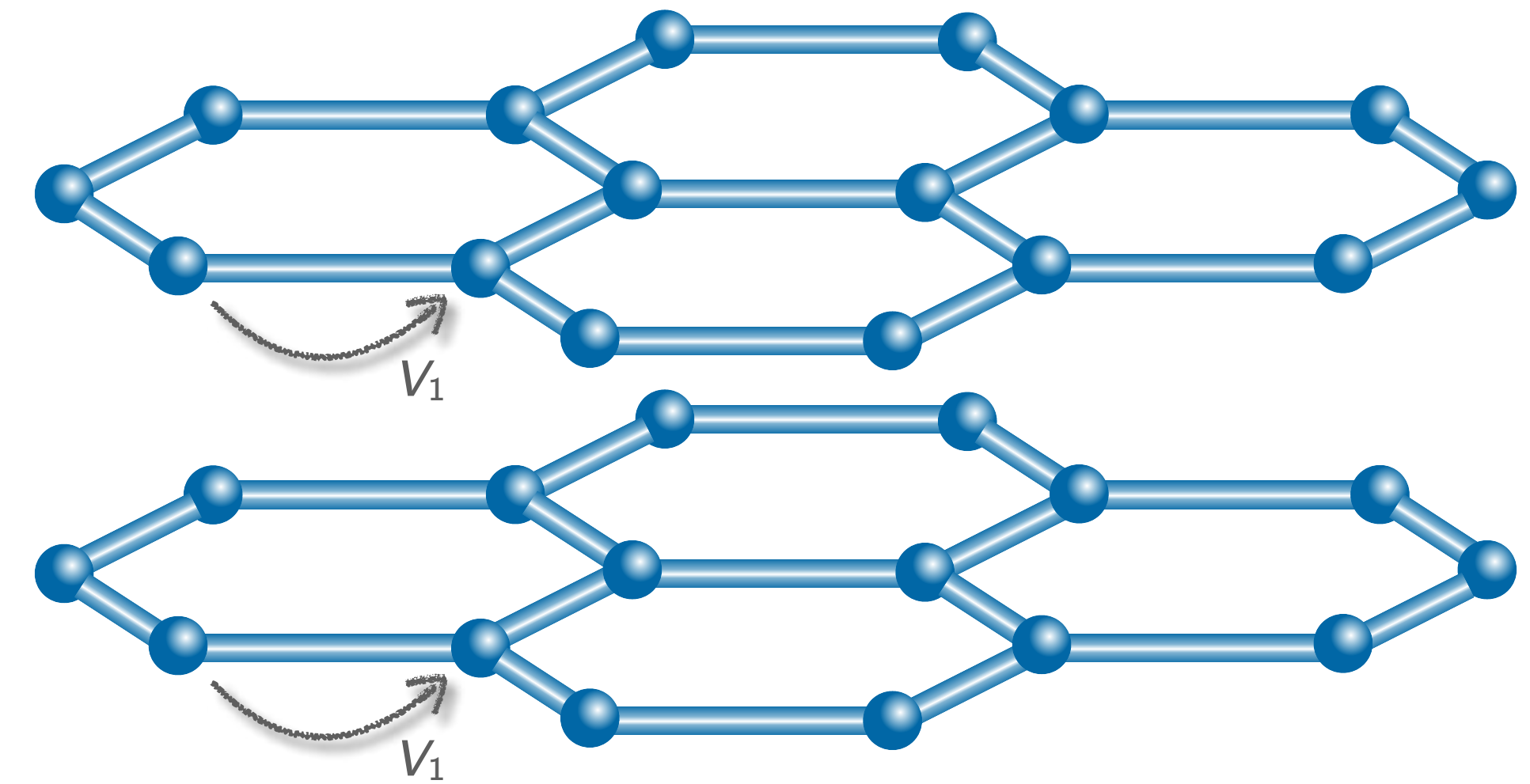
$$\mathcal{H} = \sum_{i \neq j} t(\mathbf{R}_i - \mathbf{R}_j) c_i^\dagger c_j + V_1 \sum_{\langle ij \rangle} n_i n_j$$



Interactions

Toy lattice model:

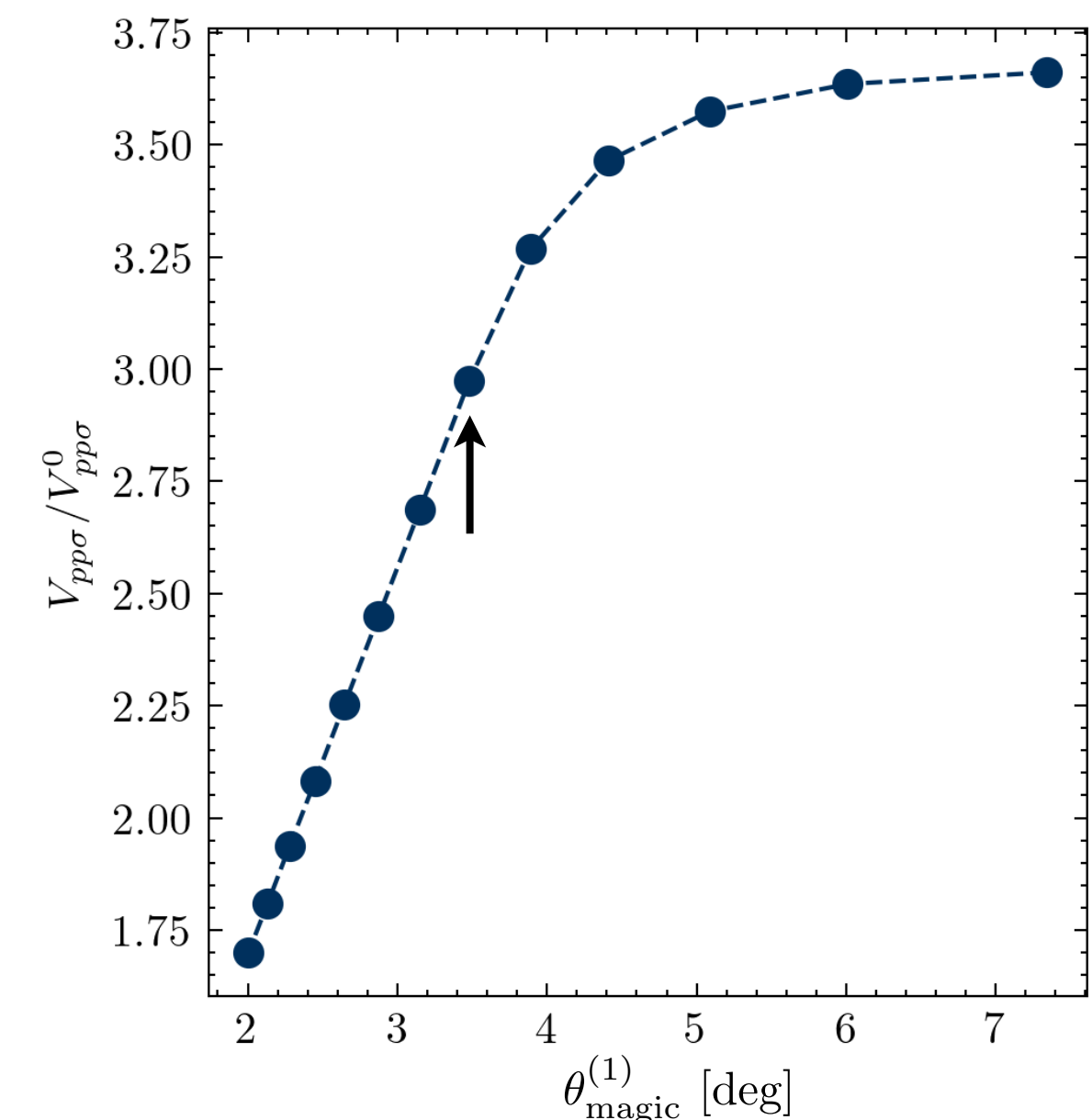
$$\mathcal{H} = \sum_{i \neq j} t(\mathbf{R}_i - \mathbf{R}_j) c_i^\dagger c_j + V_1 \sum_{\langle ij \rangle} n_i n_j$$



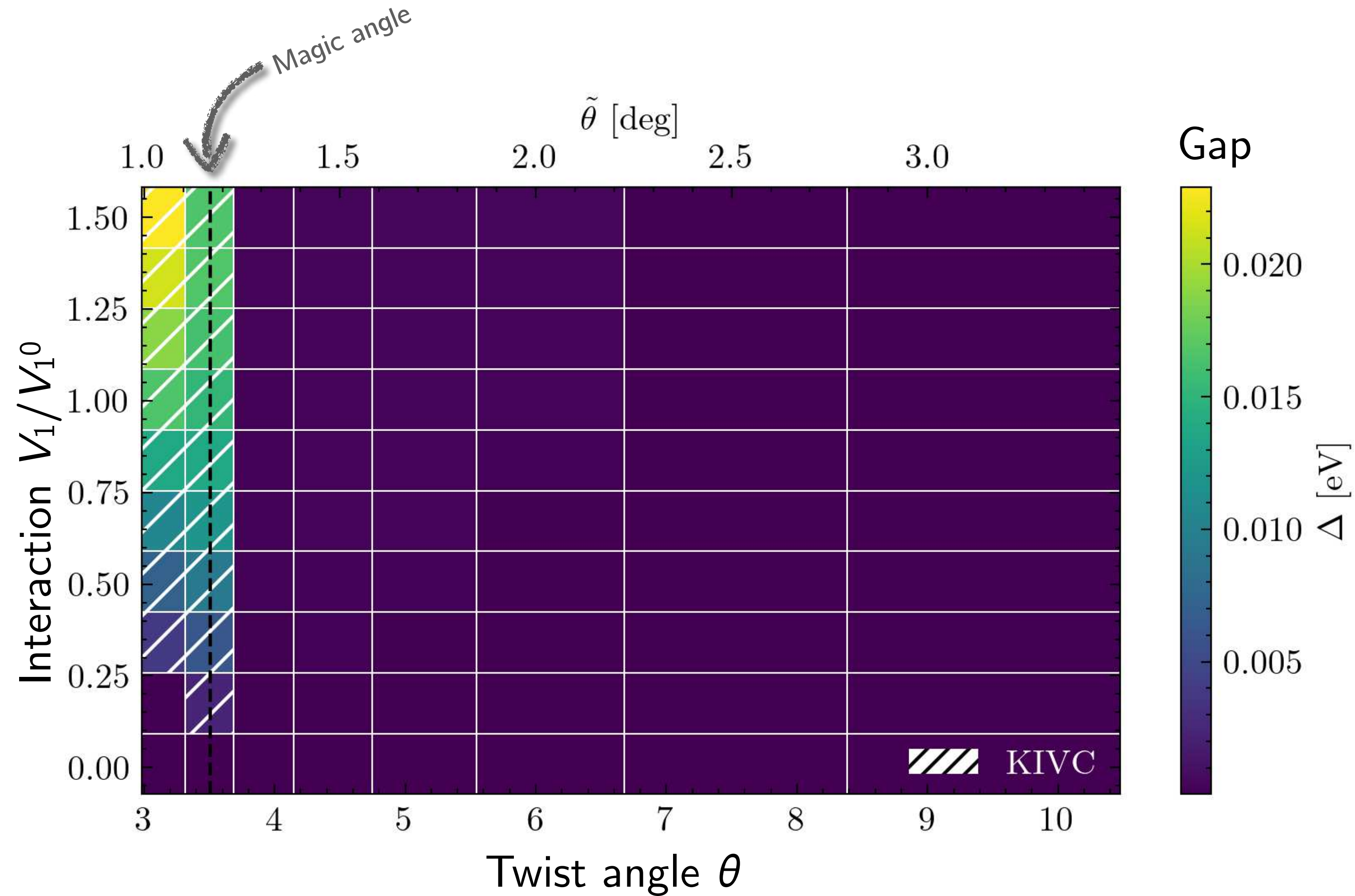
Simplifications:

- Spinless fermions
- Nearest-neighbor intralayer interactions only
- Neglect corrugation effects
- Increased interlayer hopping $V_{pp\sigma}$

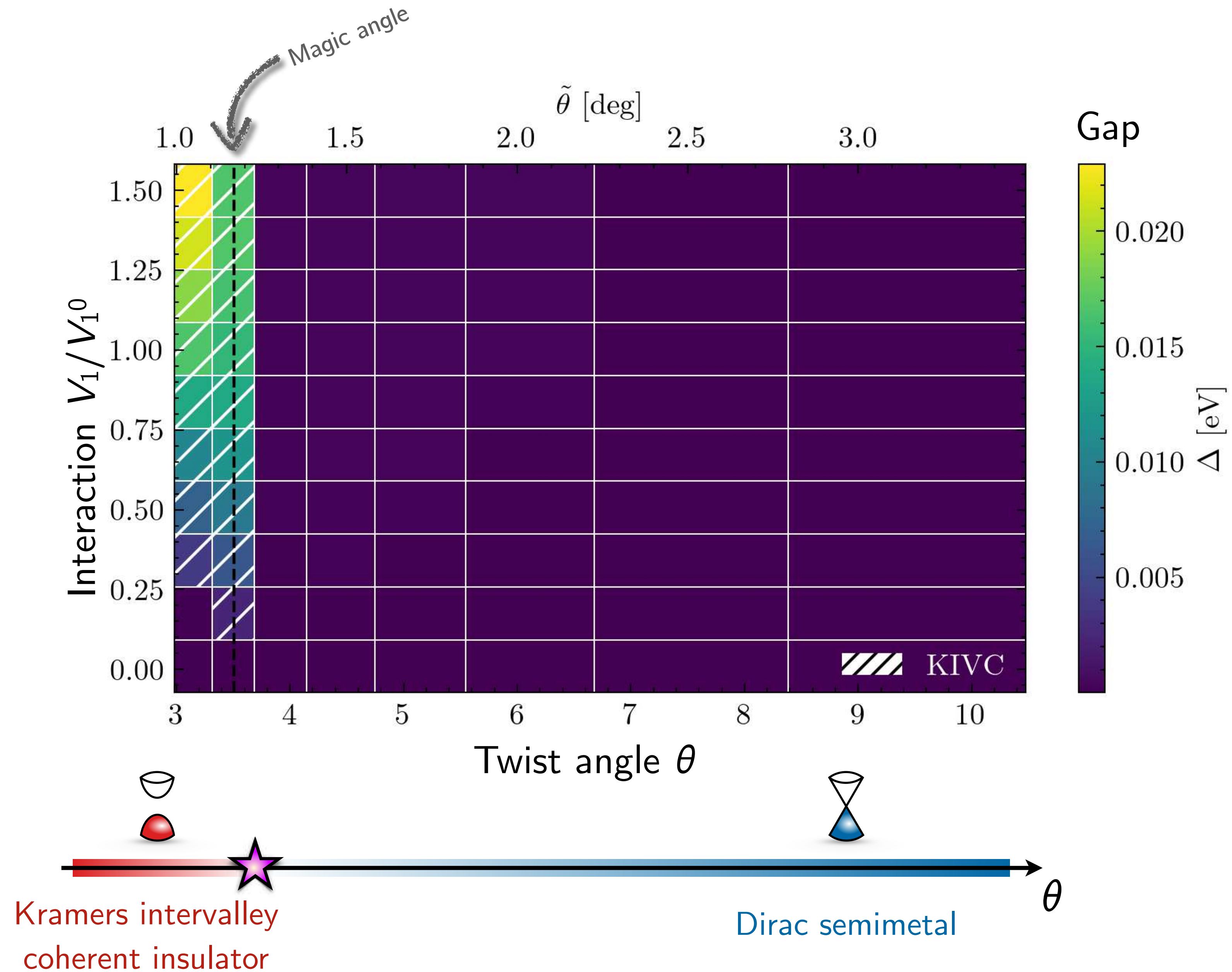
... such that $\theta_{\text{magic}}^{(1)} \simeq 3.5^\circ$



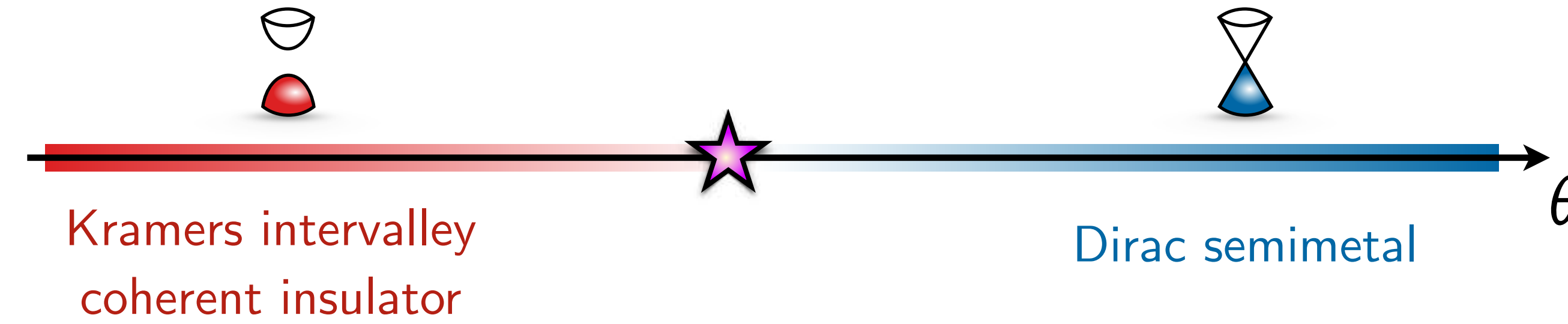
Quantum phase diagram: Mean-field theory



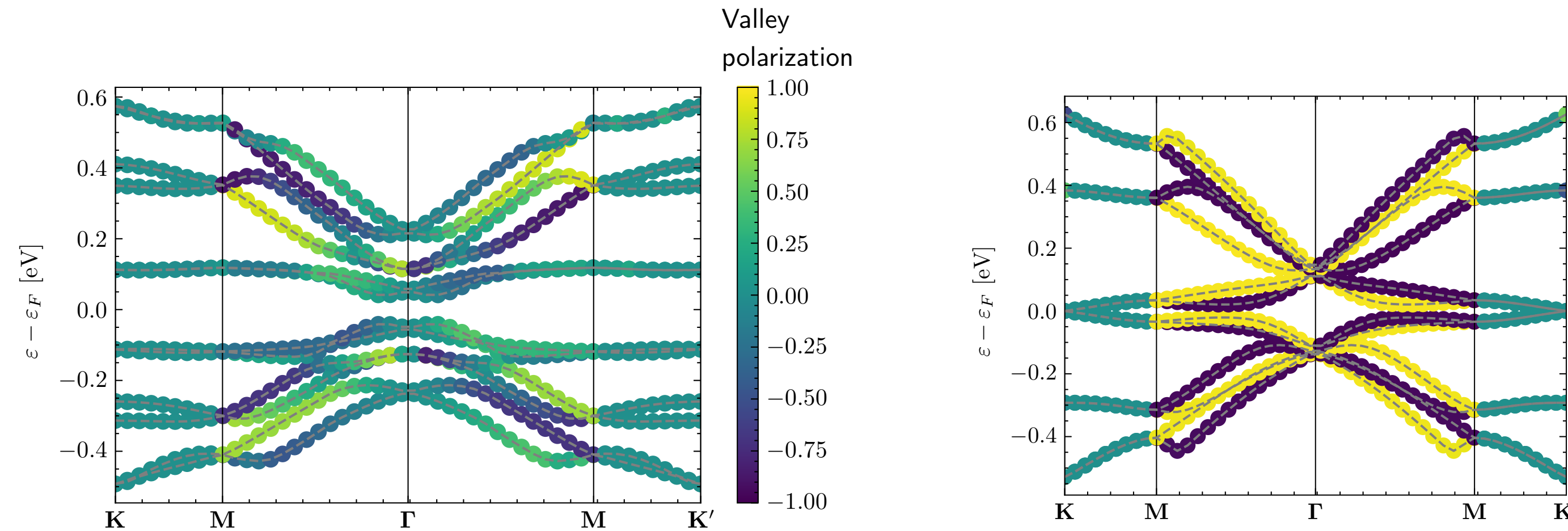
Quantum phase diagram: Mean-field theory



Twist-tuned transition



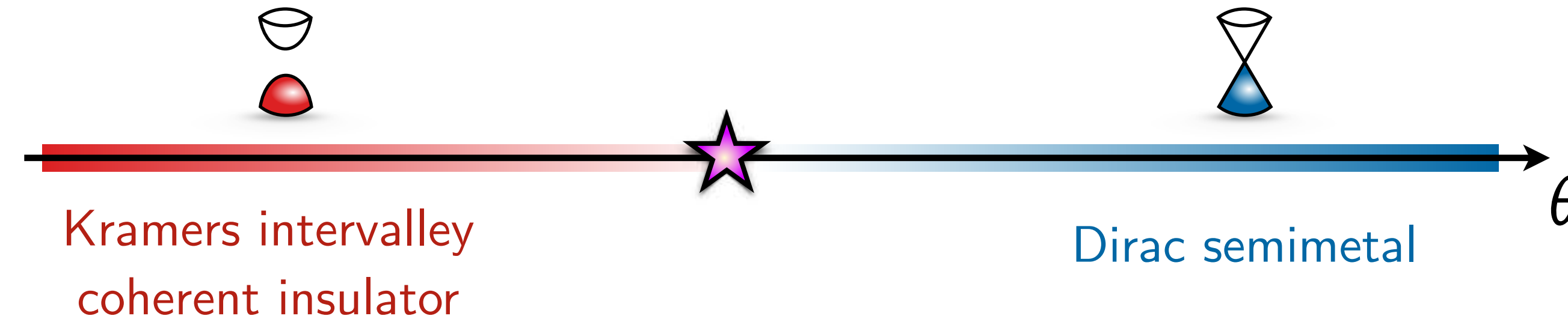
Band structure:



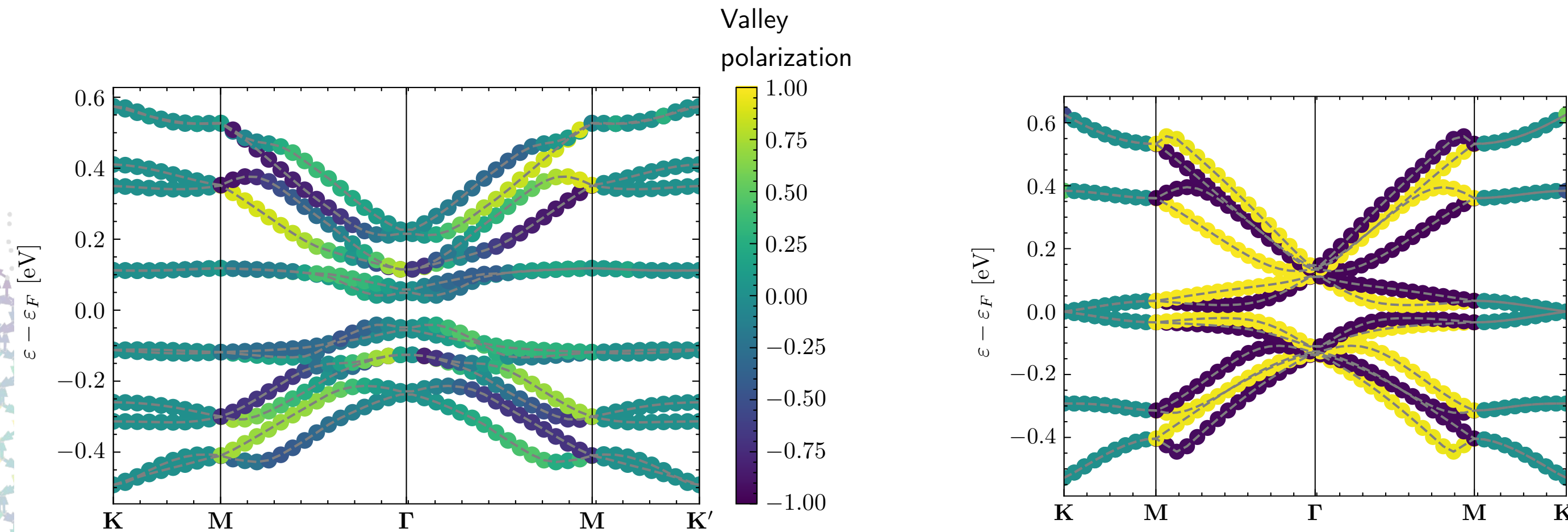
... agrees with Hartree-Fock study at $\theta = 1.1^\circ$
[Bultinck *et al.*, PRX '20]

→ Talk by R. Valentí

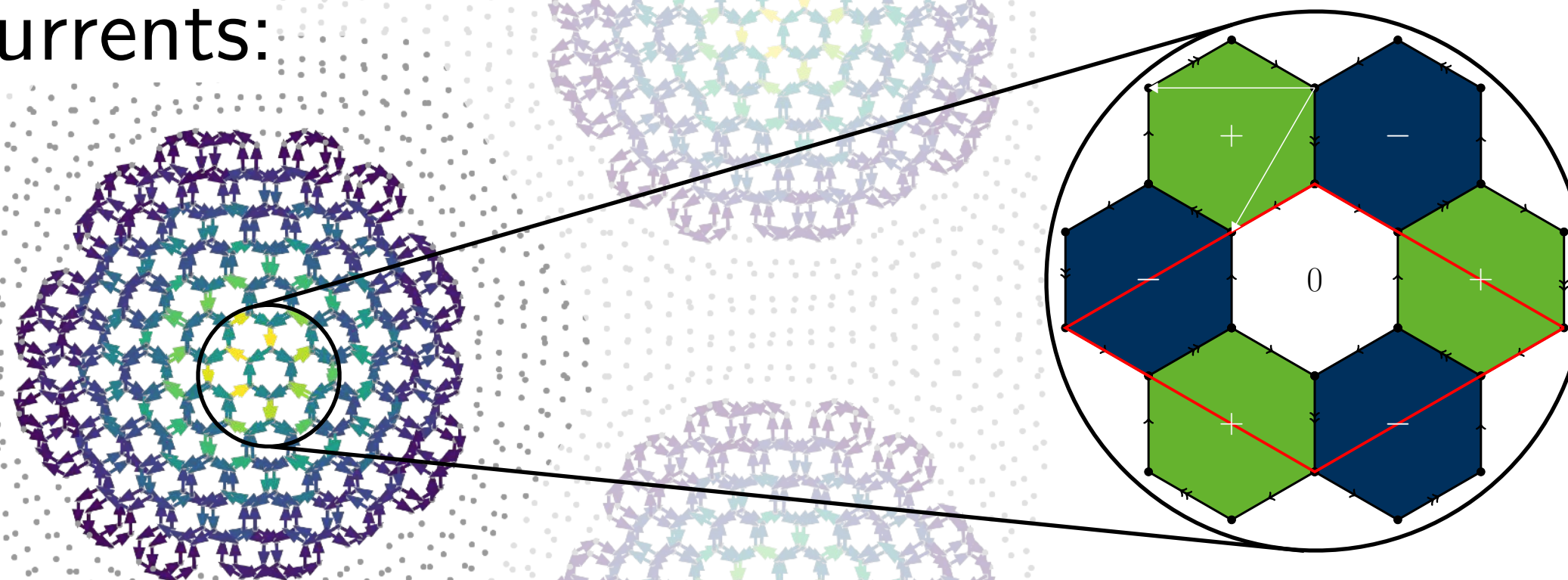
Twist-tuned transition



Band structure:



Real-space currents:

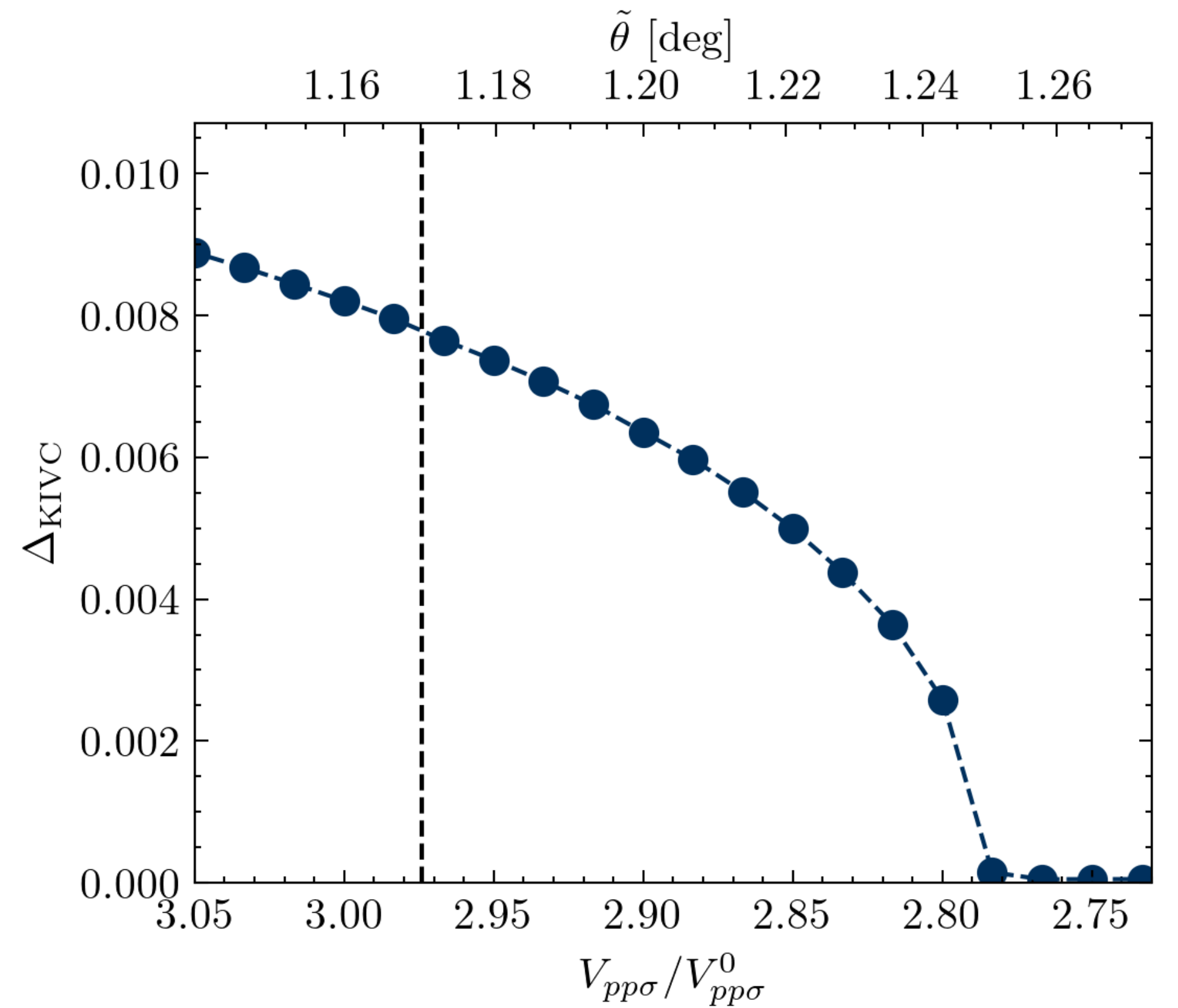


... agrees with Hartree-Fock study at $\theta = 1.1^\circ$
[Bultinck *et al.*, PRX '20]

→ Talk by R. Valentí

Twist-tuned quantum criticality

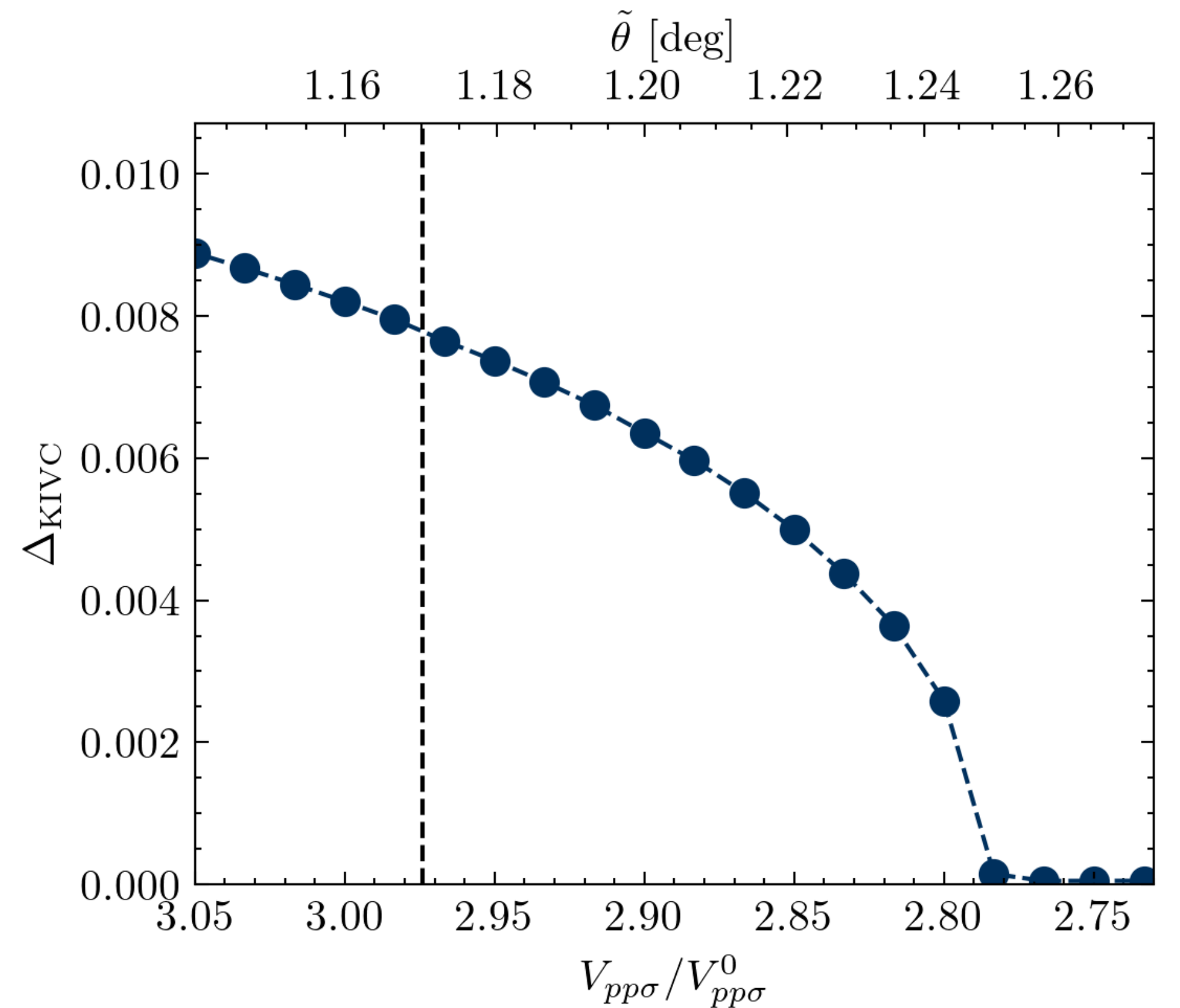
KIVC order parameter Δ vs $\tilde{\theta}$:



... for fixed $V_1 = V_1^0 = 1.45$ eV

Twist-tuned quantum criticality

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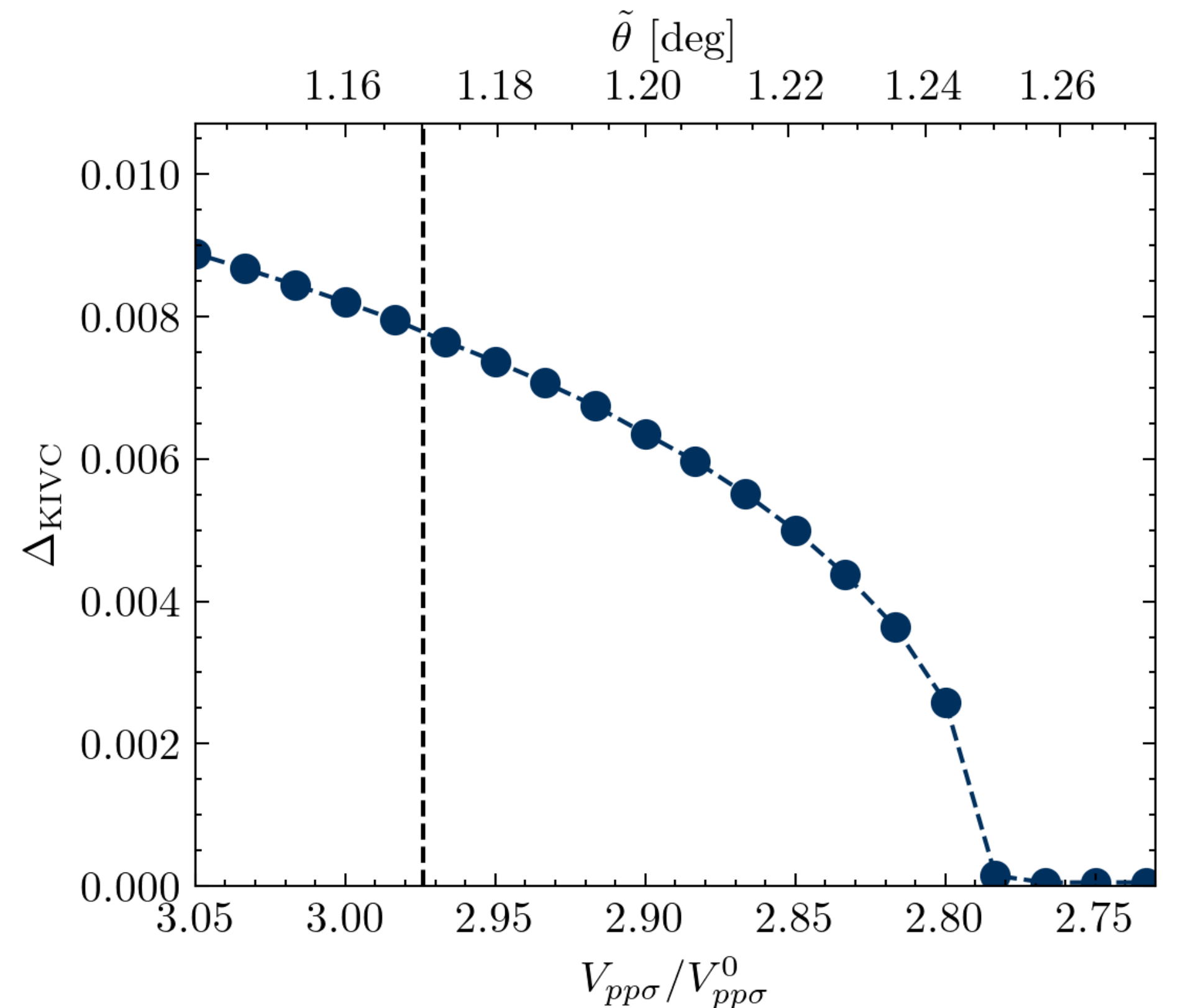
Quantum universality class:

$$\mathcal{L} = \bar{\psi} \gamma^\mu \partial_\mu \psi + g [(\bar{\psi} \gamma_3 \psi)^2 + (\bar{\psi} \gamma_5 \psi)^2]$$

... Gross-Neveu-XY

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Critical exponents:

[Gracey, PRD '21]

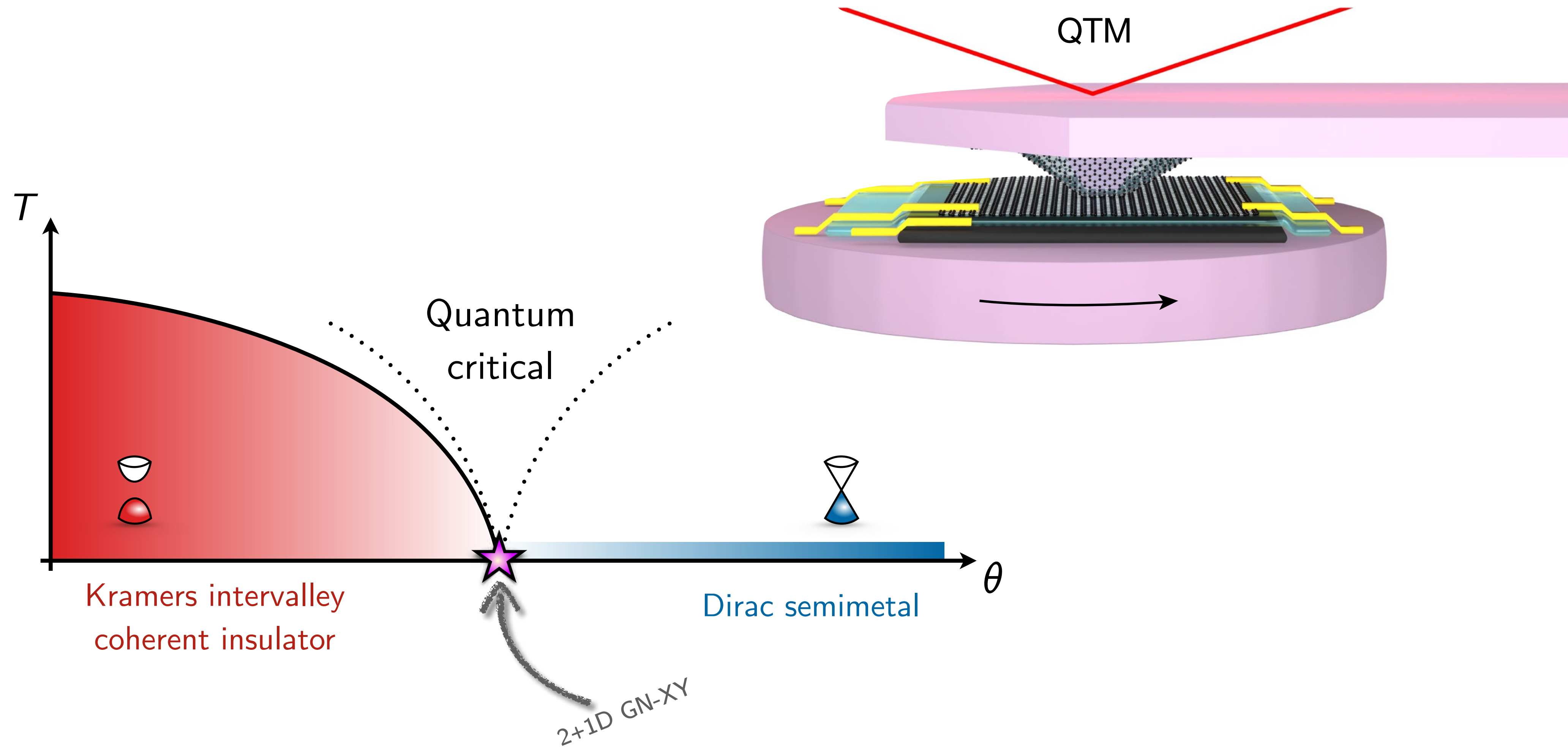
$$1/\nu = 1 - \frac{16}{3\pi^2 N} + \frac{216\pi^2 + 2912}{27\pi^4 N^2} + \mathcal{O}(1/N^3)$$

$$\eta_\phi = 1 - \frac{8}{3\pi^2 N} + \frac{544}{27\pi^4 N^2} + \mathcal{O}(1/N^3)$$

... with $N = 2$ four-component spinors (spinless fermions)
or $N = 4$ four-component spinors (spin-1/2 fermions)

[Biedermann, LJ, in preparation]

Conclusions



Candidate ground states

State of Matter	C_2	$\mathcal{T}$	$C_2\mathcal{T}$	$U_V(1)$
Semimetallic (SM)	✓	✓	✓	✓
Valley-Hall (VH)	✗	✓	✗	✓
Quantum Anomalous Hall (QAH)	✓	✗	✗	✓
Valley-Polarized (VP)	✗	✗	✓	✓
Kramers Intervalley-Coherent (KIVC)	✗	✗	✓	✗

Valley polarization

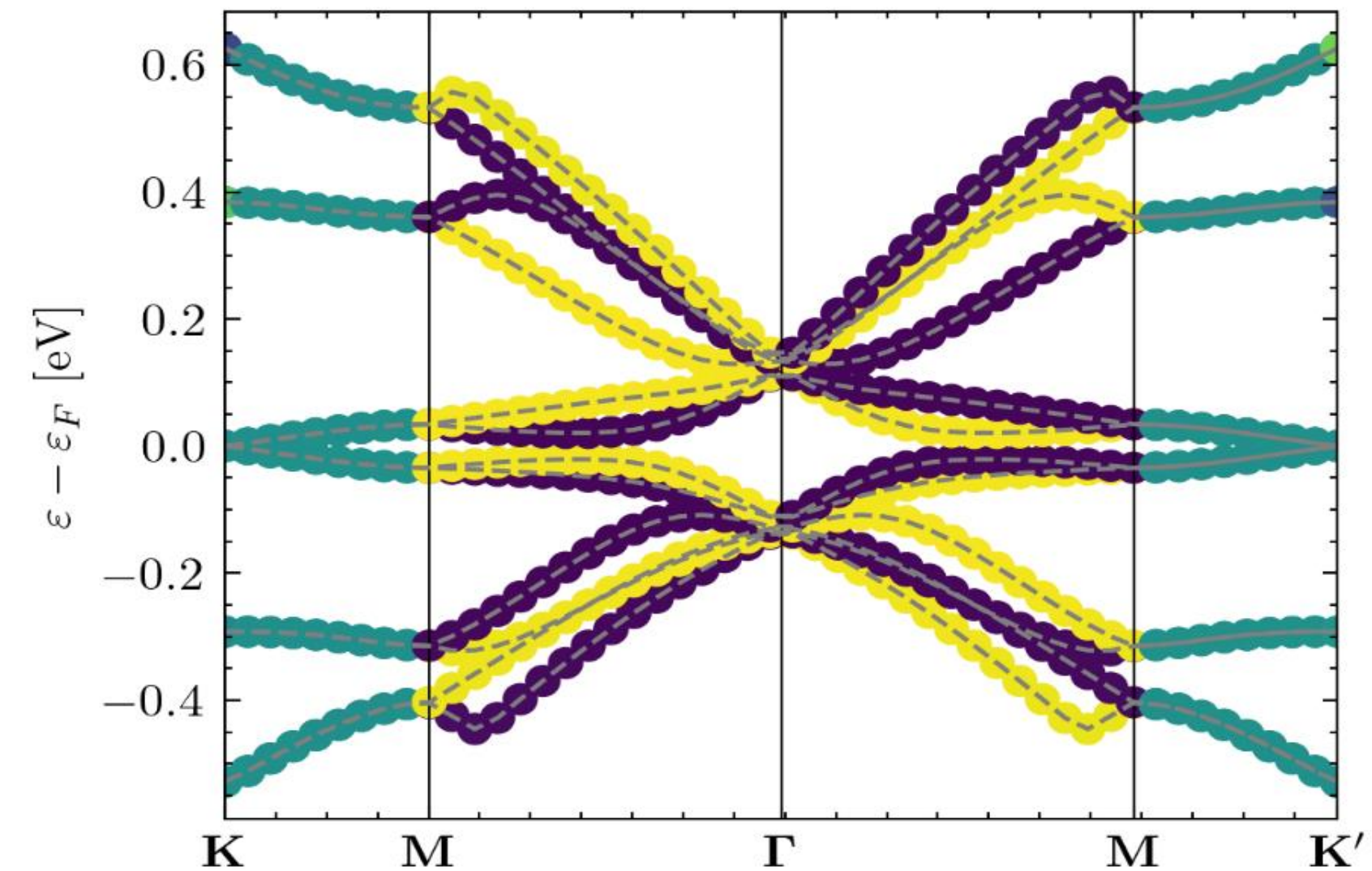
Valley polarization operator:

$$V_\ell = \frac{i}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle \in \ell} \eta_{ij} \sigma_z^{ij} c_i^\dagger c_j$$

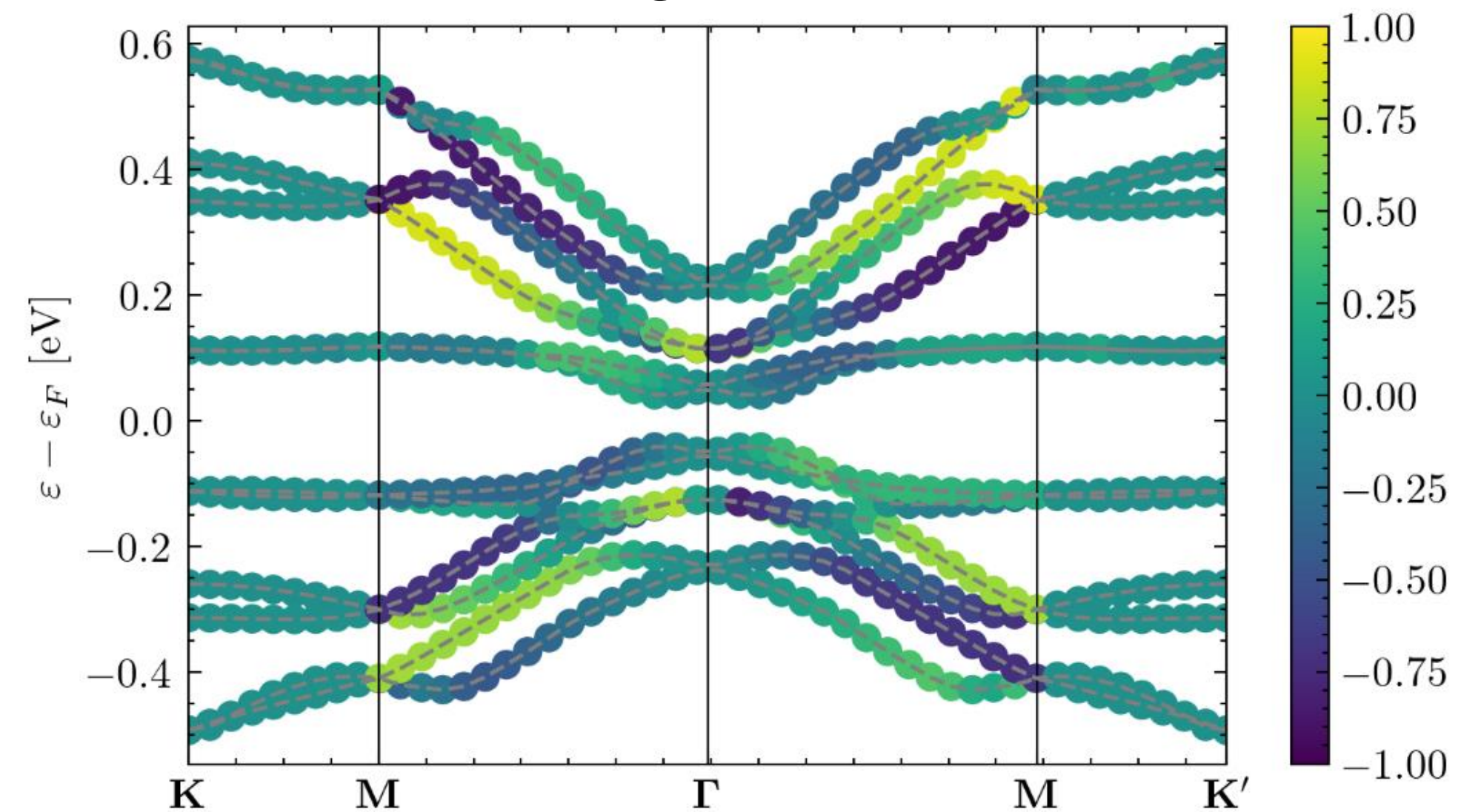
... with $\eta_{ij} = \pm 1$ for clockwise (counterclockwise) hopping

[Ramires & Lado, PRB '19]

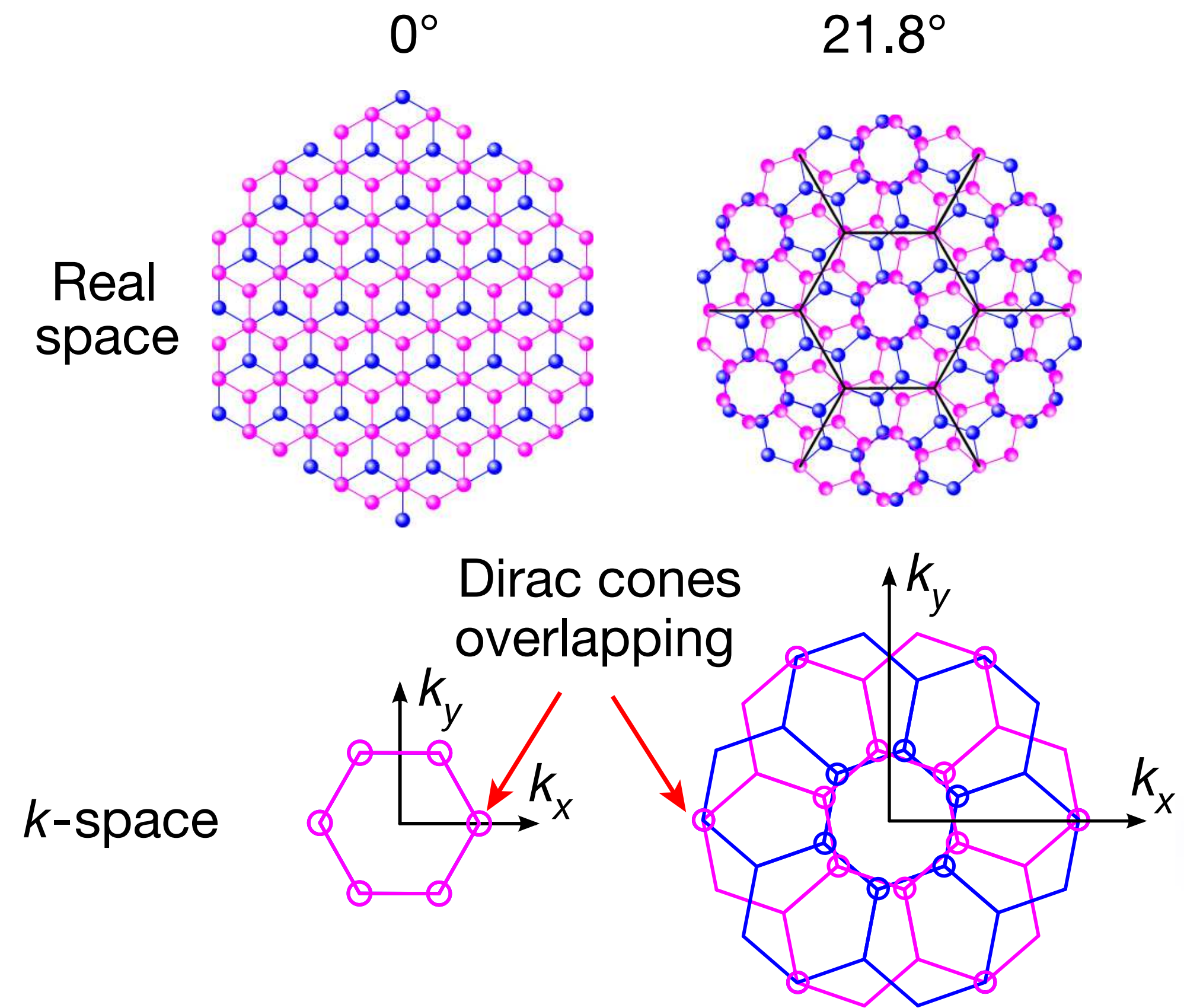
Dirac semimetal



KIVC insulator



Overlapping Dirac cones



Overlapping Dirac cones

